Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Physical Chemistry of Nanocrystals
FWP Number: KC31

Program Scope: Nanometer size inorganic crystals are playing an increasingly important role in solid-state physics, chemistry, materials science, and even biology. Many fundamental properties of a crystal (e.g., ionization potential, melting point, band gap, saturation magnetization) depend upon the solid being periodic over a particular length scale, typically in the nm regime. By precisely controlling the size and surface of a nanocrystal, its properties can be tuned. Using techniques of molecular assembly, new nanocrystal-based materials can in turn be created. This program encompasses fundamental studies of the mechanisms and kinetics of nanocrystal synthesis as well as studies of scaling laws for optical, electrical, magnetic, and structural size dependent properties.

Major Program Achievements (over duration of support): Helped develop the concept of inorganic nanocrystals as a class of macromolecule. First studies of surface derivitization and isolation of nanocrystals, and immobilization of nanocrystals on self-assembled monolayers; first photoelectron spectroscopy studies of nanocrystal electronic structure (with Jim Tobin) and nanocrystal surface structure. X-ray Absorption Spectroscopy as a tool for determining nanocrystal surface structure; first measurements of single nanocrystal x-ray absorption spectra. Synthesis and shape control of semiconductor nanocrystals and nanorods of CdSe, InP, InAs, GaAs, Co, and Fe_2O_3. Discovery of branching in nanorod synthesis of II-VI semiconductors, including synthesis of tetrapods and inorganic dendrimers. Studies of core-shell nanocrystal synthesis and properties. Optical properties of nanocrystals, including hole-burning, resonance Raman, photon echo, Stark effect; polarization and blinking studies of quantum dots and nanorods. Studies of pressure and temperature induced structural transformations in nanocrystals. Single nucleation events in nanocrystal structural transformations; shape change as an indicator of mechanism in nanocrystal transformations, first measurements of activation energy and activation volume in nanocrystal structural transformations. Hollow nanocrystal formation through the nanoscale Kirkendall effect. Cation exchange kinetics, reversibility, mechanism in nanocrystals. First electrical device based on a nanocrystal-polymer composite (light emitting diode); first transistor based on a single nanocrystal and a single molecule (with Paul McEuen); developed the use of DNA as a tool for patterning nanocrystals (with Peter Schultz); discovered liquid crystal phases of semiconductor nanorods; introduced the use of colloidal quantum dots as fluoresecent biological labels (with Shimon Weiss); first demonstrated the plasmon spectroscopic ruler for measuring nanoscale distancesHybrid nanorod-polymer solar cell. Dual Nanocrystal Solar cell

Program impact: Light emitting diodes, solar cells, solar concentrators, fluorescent biological labels (reduced photbelaching, multiplexed assays), magnetic storage, magnetic bio-labeling, mechanical reinforcement of composites. Education: About 100 scientists have been trained in the lab, and are now active in the science community. (alumni at Arkansas, Bain Consulting, Cambridge University, Exxon-Mobil, General Electric, Univ. of Hamburg, Harvard, Hebrew Univ. of Jerusalem, Intel, Univ. of Mainz, MIT Media Lab, Mitsubishi Chemical, Nanotectonica, Nanosys, Naval Research Lab, Patent Attorney, Quantum Dot Corp., Rice, National Taiwan University, Siemens, Stanford, UCLA, Vanderbilt).

Interactions: Current collaborators: Jean Frechet (Chemistry and MSD), Daniel Chemla (Physics and MSD), Alex Pines (MSD and Chemistry), Anupam Mahukar (USC), Ned Seeman (NYU), Laura Landweber (Princeton), Priya Vashista (LSU), Lydia Sohn (Princeton). Former collaborators: Chuck Shank, Peter Schultz, Paul McEuen. Industry Interactions: Founder, Quantum Dot Corporation; Founder, Nanosys, Inc.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Patents: Ten issued. Founded two companies: Quantum Dot Corporation (fifty five employees) with focus on biomedical applications of semiconductor nanocrystals, and most recently, Nanosys, with focus on electro-optic applications. Small Times 2003 Researcher of the Year. 2nd most cited scientist in nanotechnology for 1993-2003 (ISI). Press Articles**:** C&E News, Science, Nature, Science News, Scientific American, MIT Technology Review, Red Herring, Business Week, Service to the community: Founding editor-in-chief of Nano Letters (American Chemical Society); Associate Editor, Annual Reviews of Physical Chemistry; co-author with Mike Roco of the NSF and Stan Williams of HP, of the National Nanotechnology Initiative Report. DOE Council on Materials Science; External Review Board of the Joint Institute of Laboratory Astrophysics; National Research Council Solid State Sciences Subcommittee. Examples of Awards and Honors: ~30 plenary and invited lectures last year, including seven endowed lectureships; NSF Presidential Young Investigator, Sloan Foundation Fellow, Exxon American Chemical Society Solid State Chemistry Fellowship, Materials Research Society Outstanding Young Investigator, Wilson Prize, Harvard University, Fellow of the American Physical Society, Fellow of the American Association for the Advancement of Science, Visiting Professor St. John's College Cambridge, Colloid and Surface Chemistry ACS Award, elected to the National Academy of Sciences and the American Academy of Arts and Sciences.

Personnel Commitments FY2005: A.P. **Alivisatos**-PI (10%), 4 100% graduate students, 1 100% postdoctoral, visitors.

Authorized Budget (BA):
FY03 BA $415,000 FY04 BA $415,000 FY05 BA $615,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP Self-assembly of organic/inorganic nanocomposites materials
FWP #: KC31

Program Scope: Create functional materials by parallel and hierarchical self-assembly. Develop wet chemical processes by which organic/inorganic composites can be created with a high degree of control on many length scales simultaneously. By developing a comprehensive ability to pattern organic/inorganic composites, it will be possible to design complex materials in which several microscopic processes are independently and simultaneously optimized. Target functional materials with applications in energy conversion, mechanical composites, and optical/electrical devices. The team: Paul Alivisatos (inorganic nanocrystals); Jean Frechet (Polymers and Organic Synthesis); Miquel Salmeron (Spectromicroscopy) ; Lin Wang Wang (Theory); Daniel Chemla (spectroscopy) .

Major Program Achievements (over duration of support): Demonstrated the concept of hybrid inorganic-organic nanorod – polymer solar cells (Science 2002, *295*, 2425.); developed dual nanocrystal solar cell (Science 2005); General route to vertical ZnO nanowire arrays using textured ZnO seeds (Nano Lett 2005); Nanowire dye-sensitized solar cells (Nature Materials, 2005); developed new specialty electro-active surfactants that solubilize inorganic nanorods, while permitting electron transfer (Adv. Materilas 2002); calculated the energy levels of semiconductor nanorods vs. aspect ratio, and verified the prediction that the degree of polarization should change dramatically at aspect ratio of 2 (Science 2001, *293*, 1455, Journal of Physical Chemistry B 2002, *106*, 2447); discovered the existence of liquid crystal phases of inorganic semiconductor nanorods (Nano Letters 2002, *2*, 557.). Computed the energy levels of exotically shaped nanocrystals – arrows and teardrops (Nano Letters 2003); demonstrated the synthesis in high yield of branched nanocrystals(Nature materials 2003) and hyper-branched nanocrystals (Nano Letters, 2005); demonstrated the growth of nanocrystals by microfluidic techniques (Nano letters 2003, JACS 2005); demonstrated solution phase X-ray absorption spectroscopy of Co nanocrystals; Electrical and AFM investigations of individual inorganic tetrapods.

Program Impact: Examples of Applications: hybrid nanorod – polymer solar cells; light emitting diodes; mechanical reinforcement of plastics. Education: About 300 scientists have been trained in the combined labs, and are now active in the science community. (alumni at Arkansas, Cambridge University, Bain Consulting, Exxon-Mobil, General Electric, Univ. of Hamburg, Harvard, Hebrew Univ. of Jerusalem, Intel, Univ. of Mainz, MIT Media Lab, Mitsubishi Chemical, Nanosys, Covio, Naval Research Lab, Patent Attorney, Quantum Dot Corp., Rice, National Taiwan University, Siemens, UCLA, Vanderbilt). Patents: Ten issued. Founded two companies: Quantum Dot Corporation (fifty employees) with focus on biomedical applications of semiconductor nanocrystals, and most recently, Nanosys, with focus on electro-optic applications. Press Articles: C&E News, Science, Nature, Science News, Scientific American, MIT Technology Review, Red Herring, Business Week Service to the community: Founding editor-in-chief of Nano Letters (American Chemical Society); **Interactions:** Current team members: Paul Alivisatos (Chemistry and MSD) Jean Frechet (Chemistry and MSD), Miquel Salmeron (MSD); LinWang Wang (NERSC); Collaborators: Richard Mathies (Chemistry) (Daniel Chemla (Physics and MSD), Alex Pines (MSD and Chemistry), Anupam Mahukar (USC), Ned Seeman (NYU), Laura Landweber (Princeton), Priya Vashista (LSU), Lydia Sohn (Princeton). Former collaborators: Chuck Shank, Peter Schultz, Paul McEuen. Industry Interactions: 3M, Dow Chemical, Dupont, Intel, Kodak, Motorola, Xerox; Bayer, BASF, Mitsubishi Chemical, Samsung.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Alivisatos: ~30 plenary and invited lectures last year, including seven endowed lectureships; NSF Presidential Young Investigator, Sloan Foundation Fellow, Exxon, ACS Solid State Chemistry Fellowship, MRS Outstanding Young Investigator, Wilson Prize, Harvard, Fellow APS, Fellow AAAS, Visiting Professor St. John's College Cambridge, Colloid and Surface Chemistry ACS Award, elected to the National Academy of Sciences and the American Academy of Arts and Sciences. Fréchet: NAS, NAE, AAAS; ACS Award n Polymer Chemistry, Butler Lecturer Florida, ACS Salute to Excellence Award, ACS Cope Scholar Award, Baker Lecturer Cornell, Stauffer Lecturer Stanford, Bayer Lecturer, Pittsburgh, Chute Lecturer Dalhousie, Merk-Frosst Lecturer Alberta, Chambers Lecturer Rochester, Dow Karabatos Lecturer Michigan State, Doctorate (Honoris Causa) Universite Claude Bernard, France. Salmeron: Plenary lecturer 18th European Conf. on Surface Science, Keynote speaker 1st Latin American Sym. on Scanning Probe Microscopy. 13 invited talks since 2001. Yang: 2005, ACS Pure Chemistry Award

Personnel Commitments for FY2003 to Nearest +/-10%: P. **Alivisatos** (PI), M. Salmeron (senior scientist) 10%, D.F. Ogletree (staff scientist) 10%, 12 100% graduate students, 8 100% postdoctoral fellows, 2 visitors.

Authorized Budget (BA):

FY03 BA $1,394,000 FY04 BA $1,359,000 FY05 BA $1,228,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Biomolecular Materials Program
FWP Number: KC31
Program Scope: Mimicking or application of biological materials and processes in the materials sciences. Mimicking of membranes and membrane receptors for coatings and functional interactions with living cells; of carbohydrates for controlled interface properties; of proteins for nanoscale conducting wires and self-assembling building blocks for functional assemblies; of DNA and dendrimers for 3-D patterning of inorganic nanocrystals, and as components of functional assemblies.
Major Program Achievements (over duration of support): Biosensors that turn color in the presence of agents such as influenza virus, botulinum toxin (Bednarski/Charych). Development of ultrasensitive SQUID based biosensors for pathogens (Alper/Clarke). Polymers that significantly improve the stability of proteins in unbuffered solutions and at elevated temperatures (Bednarski). Development of catalytic antibodies (Schultz). Systems to insert non-natural amino acids into proteins (Schultz). The effect of specific amino acid substitutions on proteins temperature stability (Kirsch). Enzyme mechanisms for discrimination between optical isomers (Koshland). Techniques to metabolically modify cells for specific attachment to inorganic surfaces without loss of function (Bertozzi). New approach for mineralizing organic polymers and self-assembled systems with inorganic composites for tough, lightweight, fracture-resistant organic/inorganic hybrid materials modeled on bone (Bertozzi). Development of new biomimetic, carbohydrate-like polymers with lubricating properties modeled after biological mucins (Bertozzi). New technologies for endowing carbon nanotubes with biomimetic surfaces capable of interfacing with proteins and cells. Methods for isolating gold nanocrystals bearing discrete numbers of DNA oligonucleotides and the preparation of dimers and trimers of these DNA-nanocrystal assemblies and a wide variety of other spatial arrangements of nanocrystals. Discrete quantum dot Au assemblies and Au nanocrystal spectroscopic plasmon ruler (Alivisatos). A series of unnatural building blocks to enable automated preparation of self-assembling dendritic materials based on DNA base pairing (Frechet). Well defined assemblies of nanocrystals in specific arrangements (Frechet/Alivisatos). Biocompatible synthetic gels. A system to deliver biological molecules to prepatterned membrane structures using targeted membrane fusion (Groves). Modification of natural products to allow the attachment of actin fibers to inorganic surfaces for rudimentary circuit construction (Francis). Attachment of polymers and other molecules to the viral coat protein as building blocks for complex structures (Francis). Functionalization of tobacco mosaic virus coat proteins to allow the construction of linear arrays of inorganic nanocrystals (Francis). Efficient chemical strategies for the modification of protein building blocks (Francis). Activation of neurons from synthetic supported membranes and use of nanopatterned hybrid inorganic/organic membrane interfaces to repattern a synapse with a living Tcell (*Science* Nov. 18, 2005)(Groves). Application of in situ photolithographic patterning technology to membrane patterning on colloidal particles (*Adv. Mats*. 2005. Use of membrane coated colloidal particles as sensitive detection assay (*Nature* 2004)(Groves).
Program Impact: Biosensors for study by industry/government for military/civilian use. Expanded capability to modify enzymes for novel functions. Commercial product for stabilization of proteins at high temperatures and in unbuffered solutions. Techniques for creating hybrid devices of living cells and non-living materials, and for integrating nanoscale materials into biological systems. Over 10 papers/year in major peer reviewed journals.
Interactions: C. Larabell, UCSF; L. Landweber, Princeton; N. Seeman, NYU; M. Dustin, NYU; M. Callstrom, Ohio State; A. Tomsia, R. Ritchie, K. Healy, R. Mathies, E. Isacoff, LBL and UCB; A. Zettl (LBNL/UCB), Arto Nurmikko (Brown), Harry Atwater (CalTech), Angela Belcher (MIT), Rajesh Naik (AFRL), Johnathon Trent (NASA), Chad Paavola (NASA).
Recognition, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Bertozzi- Elected Amer. Acad. Arts & Sciences, Irving Sigal Young Invest. Award-Protein Society, ACS Award-Pure Chemistry, Merck Academic Development Award, Pres. Early Career Award-Science & Engineering, MacArthur Found. Award, Camille Dreyfus Teacher-Scholar Award, Arthur Cope Scholar Award ACS. *Alivisatos*-Nat. Acad. Sci. Amer. Acad Arts and Sci. ACS Colloid and Surf. Sci. Award. Fellow, AAAS, APS, Wilson Prize-Harvard, Coblentz Award, Sloan Found. Fellow, Pres.Young Investigator, Outstanding Young Invest.-MRS, Editor-in-Chief NanoLetters, Associate Ed. Ann Rev Phys Chem, Editorial Board: J Phys Chem, Chem Phys, J Chem Phys. *Frechet*-Nat. Acad Sci, Nat Acad Engin, Amer Acad Arts Sci, ACS Award-Polymer Chem, 2005 Esselen Award for Chemistry in the service to the public, ACS Salute to Excellence Award, ACS Cope Scholar Award, Baker Lecturer-Cornell, Stauffer Lecturer-Stanford, *Groves*- Searle Scholars Award, MIT TR100 (2003), Beckman Young Investigator Award (2004), ACS Langmuir Lecture Award (2005), *Francis*-Hellman Faculty Award (2004) Dreyfus Foundation Award.
Personnel Commitments for FY2003 to Nearest +/-10%:
Profs M. **Alper**, P. Alivisatos, J. Fréchet, C. Bertozzi, J. Groves, M. Francis at 10%. Staff Sci: J. Song (50%), 4 post-docs at 100%, 5 GSRAs at 100%.
Authorized budget (BA):
FY03 BA $732,000 **FY04 BA** $732,000 **FY04 BA** $732,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Many Body Processes and Quantum Size Effects in Semiconductor Nanostructures and Correlated Electron Systems
FWP Number: KC22

Program Scope: Exploration of physical properties of nanostructures and low dimensionality materials with length scales on the order of a few nanometers. Because of quantum size effects, the system properties are size and shape dependent and neither like those of atoms or macroscopic solids. Our interest in many-body and collective effects in low dimensional systems stems from the fact that in such systems quasi-particles have fewer degrees of freedom to avoid each other and hence the many body interactions become dominant. We focus on two classes of materials: semiconductor nanostructures and low dimensional strongly correlated electron systems.

Major Program Achievements:
(1) Coherence and dephasing in systems with correlated ground state: 1a- First investigation of the quantum coherence of *e-h* pairs in the presence of a two-dimensional electron gas (2DEG) in the quantum Hall effect regime. 1b- Dynamics of the inter-Landau Level excitations of a 2DEG in large magnetic fields.
(2) Exciton in Coupled Quantum Wells (CQW): Quasi-2D spatially indirect excitons in CQW have extremely long lifetime and short cooling times, thus forming an ideal system to explore degenerate Bose-gas in the solid state. 2a- First observation of buildup of highly statistically degenerate indirect excitons. 2b- First observation of macroscopically ordered exciton states, revealed by fragmentation of the ring-shaped emission pattern into circular structures forming periodic arrays over macroscopic lengths, up to 1 mm.
(3) Charge-pair correlations at meV energy scales. 3a- Ultrafast bimolecular kinetics of Cooper pair formation from quasiparticles in high-T_C superconductors. 3b- Formation of an insulating exciton state from a conducting two-dimensional gas of correlated e-h pairs studied via transient terahertz spectroscopy. 3c- First THz stimulated emission from intra-excitonic transitions observed. 3d- First measurement of intra-excitonic resonances and their THz redshift at high densities.

Program Impact: Understanding many particle systems in one of the outstanding issues of modern physics. This problem is most pronounced in condensed matter physics because here "quasi-particles" are complex objects with an internal structure, strongly interacting among themselves in the background of a "vacuum" itself dynamical and structured. Quantum size effects appear when the dimensions of a system become comparable or smaller than the characteristic lengths that govern the quantum mechanics of the process under investigation. In particular, many theoretical approaches, Random Phase Approximation, Boltzmann Kinetics, Fermi Golden Rule etc., can cease to be valid in nanoscale systems, especially on very short time scales. This opens the way for a wealth of unprecedented investigations, and provides new opportunities to test our understanding of fundamental physical processes in regimes previously inaccessible. Furthermore, properties of nanometer materials can be engineered at the atomic level to optimize their functionality for specific applications. These new and atomically designed artificial materials have the potential to revolutionize material sciences, and to produce devices with highly improved performances.

Interactions: Prof. A. Gossard, UC Santa Barbara; Prof. Y. R. Shen, Prof. G. Fleming, Prof. P. Alivisatos, UC Berkeley; Prof. L. Butov, UC San Diego; Prof. J. Eckstein, University of Illinois, Urbana-Champaign; Prof. I. Perakis, University of Crete, Greece; Prof. J. Tignon, Ecole Normale Superieure de Paris, France.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask) :
Member of the National Academy of Sciences; Fellow: Physical Society of America, IEEE-Laser and Electro-Optic Society, Optical Society of America; 1988 R.W. Wood prize of the Optical Society of America, 1995 Quantum Electronics Award of the IEEE Laser and Electro-Optics Society, 1995 Humboldt Research Prize, 1998 Gordon Conferences A. M. Cruikshank Lecturer. 2005, DOE Distinguished Associates Award.

Personnel Commitments for FY2005: Daniel **Chemla** (Group Leader) 40% (0% funding), R. Kaindl (Staff. Sci) 100%, M. Breit/J. Wang (Postdoc) 100%, R. Huber (Visiting Postdoc) 100% (66% funding), N. Nielsen (Postdoc) 100% (0% funding) I Cotoros (Graduate Student) 100% (35% funding), K. Dani (Graduate Student) 100%, B. Schmid (Graduate Student) 100% (0% funding)

Authorized Budget (BA):
FY03 BA $531,000 FY04 BA $515,000 FY05 BA $515,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and/or subtask Title under FWP: Superconductivity
FWP Number: KC22

Program Scope: Development of low-and high-transition temperature (T_c) Superconducting QUantum Interference Devices (SQUIDs) and their application to a broad range of phenomena. Low-T_c SQUIDs: nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) in ultralow magnetic fields at frequencies as low as 100 Hz; multiplexers for readout of bolometers for far infrared and submillimeter astronomy; novel microstrip resonator configuration for axion detectors and detection of quantum coherence; nondestructive evaluation of fatigue in steel after fatigue cycling or other processing techniques.

Major Program Achievements: Sensitivity of SQUID-based MRI system improved by factor of three. Substantial enhancement of relaxation-time (T_1) contrast demonstrated in MRI images of phantoms at frequencies below 10 kHz. Novel technique enables the elimination of concomitant gradient artifacts in ultralow magnetic fields. Static polarization of nuclear spins by means of a rotating magnetic field demonstrated and is in good agreement with theory. Microstrip SQUID amplifier achieved noise temperature within 20% of the quantum limit at 0.8 GHz.

Program Impact: SQUID-based MRI has been licensed for commercial development. Groups at LANL, PTB (Germany), Jülich (Germany) have constructed SQUID-based NMR and MRI systems. SQUID-multiplexers for readout of far infrared bolometers will be deployed on a 330-element array on a telescope at Atacama, Chile in late 2005. Upgrade of axion detector at LLNL to incorporate microstrip SQUID amplifier has been funded and is in progress. Microstrip SQUID amplifiers are in operation at Yale University, Chalmers University, Gothenburg, Sweden and the University of New South Wales, Australia.

Interactions: Internal: E.L. Hahn (Physics, UCB); Ben Inglis, (Brain Imaging Center, UCB); J. A.T. Lee (Physics, UCB); D-H. Lee (Physics, UCB); J.W. Morris (Materials Sciences, UCB); A. Pines (Chemistry, UCB and MSD, LBNL); P.L. Richards (Physics, UCB); H. Spieler (Physics, LBNL).

External: P. Delsing (Chalmers University, Sweden); N. Hylton (UCSF); D. Kinion (LLNL); Kurhanewicz (UCSF); M. Mück (University of Gießen, Germany); D. Reilly (University of New South Wales); R.J. Schoelkopf (Yale University); M. Shuman (UCSF); J. Simko (UCSF); K. van Bibber et al. (LLNL).

Recognitions, Honors and Awards: J. Clarke - Olli V. Lounasmaa Award, Finnish Academy of Arts and Sciences; Hughes Medal, Royal Society; Faculty Research Lecturer, University of California, Berkeley; Editorial Boards of Journal of Low Temperature Physics and Superconductor Science and Technology; Member of Solid State Sciences Committee of National Academy of Sciences (2003-2006); International Advisory Committee, International Symposium on Superconductivity (ISS), Tsukuba, Japan (2005). National Advisory Committee, 24th International Conference on Low-Temperature Physics (LT24), Orlando, Florida (2005); International Advisory Committee, 10th International Superconductive Electronics Conference (ISEC), Noordwijkerhout, The Netherlands (2005). 26 invited talks in 2005.

Personnel Commitments for FY2005 to Nearest +/- 10%:
J. Clarke (program leader) 15%; gsr's (62.5%): S-K. Lee (graduated 5/05), W. Myers, N. Kelso, M. Hatridge (started 6/05), S. Busch (started 7/05); postdocs (100%): D. Kinion (zero time charged to project), M. Moessle; admin. (charged to project 50% of year) (75%): B. Salisbury.

Authorized Budget (BA):
FY03 BA $398,000 FY04 BA $303,000 FY05 BA $410,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020203

FWP and possible subtask under FWP: Quantum Theory of Materials
FWP Number: KC23

Program Scope: Theoretical calculations are employed to further the basic understanding of the physical properties of materials and materials systems. The emphasis is on carrying out quantum-mechanical calculations for realistic systems based on microscopic first-principles approaches. Model systems are also examined, and new theoretical techniques are developed. Studies include bulk materials, fullerenes, nanotubes, superconductors, surfaces and chemisorbed systems, materials under high pressure, two-dimensional electron systems, polymers, clusters, and defects in solids. Close collaboration with experimentalists is maintained.

Major Program Achievements (over duration of support): Explained properties of materials (e.g., bonding and structural properties; band structure and optical properties; properties of defects, surfaces, clusters and nanostructures) and predicted new materials and phenomena (e.g., superhard materials, new class of nanotubes, new phases of materials under high pressures, new superconductors). Developed theoretical and computational methods (e.g., empirical and ab initio pseudopotential methods, supercell technique, total energy method for structural properties, many-body Green's function approaches for spectroscopic properties, quantum Monte Carlo methods for electron correlations, NMR studies, and forces in excited states.) Recent highlights include calculations of electronic and optical properties of nanostructures, design of group IV semiconductor alloys, multigap superconductivity in MgB2, optical properties of surfaces and polymers, ideal strength of materials, photoemission and electronic properties of C60, quantum computation, and transport through single molecules.

Program Impact: Led to new discoveries, explanation of experiments, and development of methods. Advances of major impact include systematic unraveling of optical and photoemission properties of semiconductors; determination of surface/interface structures and properties; calculation and prediction of structural phase transitions; solution to the band gap problem; quantum Monte Carlo studies of real materials; prediction of superconductivity, superhard materials and new nanotubes. The theoretical and computational methods (discussed above) developed have become standard tools in the field and are being used by researchers worldwide. Many of the former students and postdocs are now leaders in the field in academia, industry and national laboratories.

Interactions: Internal—NERSC/LBNL (Canning, Meza, Wang), MSD/LBNL (Chrzan, Crommie, Morris, Zettl), CSD/LBNL (Fleming, Head-Gordon); UC Berkeley Center for Integrated Nanomechanical Systems; External—U of Minnesota; U of Washington; Palo Alto Research Center; LLNL; Georgia Tech, Penn State, U of Texas at Austin; International—Tokyo Institute of Technology; Seoul National University; Korea Advanced Institute of Science; Taiwan National Center for Theoretical Science; IU. Pais Vasco (UPV/EHU), Spain.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
M. L. Cohen – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; APS Buckley Prize; DOE Outstanding Accomplishment in Solid State Physics Award; DOE Sustained Outstanding Accomplishment in Solid State Physics Award; APS Lilienfeld Prize; U.S. National Medal of Science; ISI's top 100 most-cited physicists; President of the American Physical Society; member of American Philosophical Society; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Harvard University Loeb Lecturer; University of Montreal Doctorat Honoris Causa; 43 invited talks since 2003.
S. G. Louie – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; DOE Sustained Outstanding Research in Solid State Physics Award; APS Aneesur Rahman Prize; APS Davisson-Germer Prize; ISI's top 100 most-cited physicists; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Outstanding Overseas Chinese Award; 48 invited talks since 2003.

Personnel Commitments for FY2005 to Nearest +/- 10%:
Principal Investigators (Cohen 25%, Louie 20%); Visiting Scientists [R. Capaz (fellowship), B. Liu (Fellowship)]; Post Docs (F. Giustino 50%; P. Zhang 50%); Grad students (J. Moussa 50%, E. Kioupakis 50%; W. Luo 50%)

Authorized Budget (BA):
FY03 BA $234,000 FY04 BA $234,000 FY05 BA $234,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020601

FWP and possible subtask under FWP: Characterization of Functional Nanomachines

FWP Number: MSD-NAN002-02

Program Scope:
Development and application of controllable, operational nanomachines and nanomotors from molecular building blocks. Determination and control of the mechanisms of chemical-to-mechanical energy transfer in naturally occurring molecular biomotors, artificial biomotors, and engineered biochemical assemblies. Chemical synthesis of new molecules having tailored geometry, electro-activity, and surface reactivity for use as nanomachine components. Local probe study of functional molecules adsorbed to surfaces and actuated using optical and electronic stimulous. Use of combined MEMS technology and fullerene growth techniques to create electro-mechanically actuated molecular motors from carbon nanotubes. Theoretical prediction and explanation of nano-motor behavior through *ab initio* electronic structure calculations.

Major Program Achievements (over duration of support):
Detailed characterization of friction and dissipation of interlayer nanotube bearings. Exploitation of nanodroplet surface tension for nanomotor drive mechanism. Progress toward scalable silicon-compatible nanotube technology. Development of a light-activated ionotropic glutamate receptor (LiGluR), an ion channel that functions as an optically controlled and powered molecular machine. Characterization and control of molecular rotational properties of individual functionalized molecules at a surface. Control of molecule-surface coupling through modification of molecular ligands and surface layers. LDA calculations performed to predict excited state induced conformational changes in adsorbed azobenzene molecules. Determination of new mechanisms for mechano-chemical transduction in the packaging motor of bacteriophage phi29, directional translocation on DNA by the protein machine FtsK, and supercoiling action of *E. coli* gyrase.

Program impact:
Fabrication and operation of remotely controlled nanotube-based mechanical motors capable of operation at high and low temperature and in UHV environment. Control of molecular nanomechanical and self-assembly behavior at surfaces. Theoretical understanding of mechanical energy dissipation mechanisms (friction) in nanotube bearings. Significant progress in characterizing and re-engineering naturally occurring molecular machines and biomotors.

Interactions:
Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory
External: IBM Almaden, Yale, University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, SUNY Stony Brook, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
A. Zettl - R & D 100; **M. L. Cohen** - National Medal of Science, APS President; **Carlos Bustamante -** Honorary Degree Doctorate by the University of Chicago**; J Frechet** - 2005 Esselen Award for Chemistry at the Service of Society; **S.G. Louie** - National Academy of Science, Outstanding Overseas Chinese Award; **D. Trauner** - Novartis Young Investigator Award

Personnel Commitments for FY2005 to Nearest +/- 10%:
1 Principal Investigator (Crommie (35%))
6 faculty scientists (Bustamante (15%), Cohen (10%), Frechet (15%), Louie (10%), Zettl (20%), Trauner (20%))
5 postdocs (A. Kirakosian (50%) R. Case (100%), T. Hugel (10%), P. Zhang (50%), S. Aloni (50%))
6 grad. students (M. Comstock (100%), K. Sivula (35%), A. Murphy (100%), G. Begtrup (60%), J. Sau (50%), M. Volgraf (100%))

Authorized Budget (BA):
FY03 $800,000 **FY04** $647,000 **FY05** $939,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020203

FWP and possible subtask under FWP: Center for X-Ray Optics subtask of Condensed Matter Physics
FWP Number: KC23

Program Scope: The Center for X-Ray Optics (CXRO) pursues core programs to address national needs in the technical areas of high-spatial and high-spectral resolution applications of electromagnetic radiation in the soft x-ray and extreme ultraviolet regions of the spectrum. CXRO builds innovative systems and instruments in this region for a wide range of scientific and technological applications in collaboration with other organizations. Elements of the program consist of ultra high-resolution x-ray microscopy/tomography, spectroscopy, interferometry, Fourier optics, techniques of modern optics, and soft x-ray coherence measurement, generation, and theory. CXRO has developed significant nanofabrication expertise to support experimental activities.

Major Program Achievements (over duration of support):
CXRO's full field x-ray microscope continues to deliver the world's best resolution 2-d and 3-d images using state-of-the-art diffractive optics, with a resolving limit of better than 15nm half pitch lines and spaces, for studies of magnetic materials, life sciences samples, and environmental/remediation. An innovative method for making diffractive elements, such as zone plates, has been developed which goes beyond lithographic limits imposed by dense line proximity effects. The technique uses unique CXRO electron beam lithography with very accurate overlay (<2 nm) to produce narrow, high aspect ratio structures which open new paths to a combination of high spatial resolution (<10 nm) and high efficiency. A new method of testing the optics has been developed and proven. New deposition techniques for reflective gratings have been developed to reduce scattering and increase efficiency, essentially increasing available coherent flux a factor of four. CXRO continued development of innovative optics (XOR patterns) for soft x-ray absorption and phase shifting material measurements of the f1 and f2 scattering factors, and is now using the CXRO new undulator beam-line dedicated to coherent science for these experiments. New multiplayer mirrors have achieved world record normal incidence soft x-ray reflectivities, and new broad band width multilayer mirrors have been demonstrated to support future femtosecond and attosecond materials probing experiments.

Program Impact:
Since being established in 1983, CXRO has been a world leader in the development and applications of high-resolution x-ray optics, including nanofabrication of diffractive optics. X-ray microscopy studies of magnetic materials are having an impact on the understanding of complex and technologically significant material interactions. Optimization of the XM-1 microscope has been completed for probing magnetic material properties at 10 nm spatial resolution and with new Fourier optical techniques. Soft x-ray microscopy and nano-tomographical studies of biological samples, funded by NIH but using XM-1, has led to the funding of a new (XM-2) microscope for the quantitative study of protein expression. Scattering coefficients (both real and imaginary) have been measured with high-accuracy near absorption edges using a new interferometric technique. The CXRO maintained database of scattering factors, available online, is heavily used (16k hits/month) by researchers throughout the world.

Interactions:
CXRO has numerous interactions with university, national laboratories, and industry, including: U. Colorado, Colorado State, U. Oregon, U. Washington, Stanford, SUNY Albany, Drexel U., U. Wuerzburg, U. Gottingen, UCSF, LLNL, SSRL, Argonne, Intel, HP, Shipley, IBM, AMD, Motorola, Max Planck.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask). 0

Personnel Commitments for FY2006:
Scientific Staff, David Attwood, 35%, Erik Anderson, 25%, Peter Fischer**,** 100%, postdoc, 100%, Eric Gullikson**,** 10%. **Matrix Labor**, Engineering/technical/computer support 3 FTE.

Authorized Budget (BA):
FY03 BA $1,788,000 **FY04 BA** $1,788,000 **FY05 BA** $1,718,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020101

FWP and possible subtask under FWP: Crystallography of Microstructures (sub-task: New Al-Si-Ge Alloys for Automobile Applications)
FWP Number: KC11

Program Scope: Investigate the fundamental features that underlie the evolution of microstructures in solids by applying crystallographic techniques to the analysis of topology and defects in crystalline materials. Understand and ultimately gain control of the structure, distribution and shape of defects such as inclusions, grain boundaries, domain walls and dislocations by establishing the basic relationship between crystallographic variables and structural observables. Such relationships are put to use both analytically, to examine the structure of defects, and synthetically, to produce new and unique microstructures with defect configurations reflecting composite symmetries. Because of the scale and nature of such microstructures, electron microscopy is an integral part of these investigations, as an analytical tool as well as a subject of technique development.

Major Program Achievements (over duration of support):

Combining high resolution Z-contrast imaging with analytical electron microscopy, we have found that precipitates in Al-(Zr,Sc) alloys form core-shell structures, with a Zr-rich shell and a Sc-rich core, both with the L12 structure. Depending on heat treatment, the particles take spherical, cuboidal or dendritic forms. It is likely that the Zr-rich shell is due to a difference in diffusion rates and acts to stabilize the particles against coarsening.

The composition of Si-Ge precipitates in ternary Al-Si-Ge alloys was determined by energy-dispersive X-ray analysis. Despite equal atomic volumes in the alloy, the composition of the precipitates was found to be enriched in Si. This observation was confirmed by thermodynamic calculations using CalPhad to predict the ternary phase diagram.

We have reported the first direct observation of size- and shape- dependent premelting at interfaces in materials. Using grain boundary allotriomorphs as single crystal particles with variable interface structure, it was possible to show that premelting depends on both, the structure of the interface and the size of the inclusion. Premelting by as much as 17°C below the bulk melting point was observed directly by in-situ transmission electron microscopy on nanoscale Pb particles at grain boundaries in Al.

Brownian motion of nanosized liquid Pb inclusions trapped on dislocations in Al thin foils was studied by in-situ electron microscopy by following the nanoscale motion of individual inclusions. Quantitative analysis shows that the 1D random motion along the dislocations is constrained by interaction between inclusions. Our analysis suggests that the mobility of the free and trapped inclusions is controlled by the kinetics of interfacial processes.

Program Impact:
This work has led to an improved understanding of the key role played by interface structure in the evolution of microstructures. In particular, the role of crystallographic alignment and confinement in a solid matrix on the behavior of nanoscale particles has been elucidated and utilized in thin film growth and precipitation reactions.

Interactions:
CEA Grenoble, Dept. Recherche Fondamentale sur la Matière Condensée (F. Lançon)
University of Copenhagen, Oersted Lab (E. Johnson)
University of Belgrade, Dept. of Materials Science (V. Radmilovic)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
26 Invited talks since 2001
Personnel Commitments for FY2004 to Nearest +/-10%:
U. **Dahmen** (group leader) 40%, V. Radmilovic (staff scientist) 100%, L. Zhang postdoc) 100%, A. Tolley (visiting researcher) 50%.

Authorized Budget (BA):
FY03 BA $204,000 FY04 BA $204,000 FY05 BA $204,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP:
Surface, Interface & Nanostructure Studies Using Novel Synchrotron Radiation Methods and Instrumentation
FWP Number: KC22

Program Scope:
This program develops and utilizes advanced techniques based upon third-generation synchrotron radiation (SR), including core and valence photoemission, x-ray absorption, and soft x-ray emission/inelastic x-ray scattering, together with complementary methods (e.g. LEED, STM, and atomic-resolution TEM), to study the atomic structures and electronic and magnetic properties of surfaces, interfaces, and nanostructures, as well as strongly correlated materials exhibiting nanoscale heterogeneity. Systems studied include: multilayers composed of metals, insulators, and semiconductors; interface effects on giant magnetoresistance (GMR), tunnel magnetoresistance (TMR), and exchange bias; temperature variation of electronic structure and magnetic order in the colossal magnetoresistive oxides; and kinetics and structure in surface reactions on metals and semiconductors. Depth-resolving spectroscopies excited by soft x-ray standing waves and sub-Angstrom holographic structural probes have recently been developed by our group, and are in use in these studies. Experiments at the Advanced Light Source make use of unique experimental capabilities, including a multi-technique spectrometer/diffractometer located on an elliptically polarized undulator, and a next generation high-speed detector for photoelectrons. There is also a strong coupling to theory, particularly for the interpretation of diffraction and holography experiments, as well as x-ray optical effects on spectroscopy.

Major Program Achievements (over duration of support):
We have continued the development of a new soft x-ray standing wave method for spectroscopically studying buried layers and interfaces in nanostructures and applied it to GMR and TMR interfaces of relevance to spintronic applications. This technique permits determining depth-resolved profiles of compositions, magnetizations, and densities-of-states in multilayer nanostructures. We have also used multiple SR spectroscopies to study the high-temperature behavior of colossal magnetoresistive oxides (e.g. $La_{1-x}Sr_x MnO_3$), observing dramatic electron localization effects. We have significantly improved the instrumentation and detectors available for both spectroscopic and x-ray holographic studies at the ALS. A new high-speed electron detector capable of operating at up to 100x the rates of present detectors has been installed at the ALS and has successfully taken data.

Program impact:
Major impacts include: developing a new and broadly useful standing-wave method for studying buried interfaces in nanostructures via the soft x-ray spectroscopies (photoemission, x-ray emission, x-ray absorption); establishing a better understanding of the high-temperature electronic structure in the CMR materials; and developing ultrahigh speed detectors for synchrotron radiation research to enable the next generation of such studies.

Interactions:
Internal: LBNL (C. Booth, P. Fischer, Z. Hussain, J. Kortright, R. Ramesh, M. Salmeron, M. Van Hove--now Hong Kong City University); External: LLNL (S. Marchesini, A. Szoke); ANL (J. Mitchell—DOE CSP in Spintronic Oxides); PNNL (S.A. Chambers); University of California-Davis (K. Liu,W. Pickett,); IBM Almaden (S.S.P. Parkin); Univ. of the Basque Country (F. Garcia de Abajo); Univ. of Tokyo (T. Ohta); Correlated Electron Research Center, Japan (Y. Tokura and Y. Tomioka); RIKEN Laboratory, Japan (M. Watanabe); Hirosaki Univ., Japan (Y. Enta); Technical Univ. of Munich (D. Menzel); Hungarian Academy of Sciences (G. Faigel, M. Tegze).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Fellow of the Institute of Physics (‘04); AVS Medard W. Welch Award (‘05); Helmholtz-Humboldt Research Award (‘05); 17 invited talks at national or international conferences or summer schools over 2003-2005.

Personnel Commitments for FY2005 to Nearest +/- 10%:
C.S. **Fadley** (50%), M. West (25%), M. Press (15%), B. Sell (50%)

Authorized Budget (BA):
FY03 BA $378,000 FY04 BA $393,000 FY05 BA $300,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Plastic Electronics
FWP Number: KC31

Program Scope:
This program is aimed at the development of the fundamental understanding of the molecular and physical principles that govern the design of novel materials for organic or plastic electronics. The program aims at the exploration of newly designed materials, the determination of their physical and functional properties, and the comparison of these properties with those of known materials to provide access to a better understanding of the design rules and structure-property relationships for this important family of energy related materials. Based on novel design concepts the synthesis of new organic molecules, oligomers and polymers with interesting electrical and optical properties will be explored. The novel materials will then be fully characterized and studied for their electrical and functional properties. Experimental methods for the control of microstructure and morphology, particularly in thin films will be developed with the aid of scattering and a variety of microscopy tools including atomic force microscopy and transmission electron microscopy. Finally the newly designed materials will undergo functional testing in model configurations in transistors, light emitting diodes, photovoltaics, etc.

Major Program Achievements (over duration of support):
Since the inception of this program earlier this year we have already realized major advances in the development of electroactive oligomers capable of self-assembly that can be used as monolayer channels in printed field-effect transistors for use as monolayer transistors. We have also developed totally novel bipolar electroactive copolymers for light emitting diodes and have demonstrated their use in highly efficient polymer-based light emitting diodes achieving over 10% front face external efficiency. Current work explores novel designs of copolymers with electron and hole transporting blocks based on fullerene and conjugated polymer chemistry as well as conjugated rod-coil block copolymer. These bipolar polymers as well as polymer nanotubes hybrid structures show great promise in the photovoltaic field. We have also elucidated mechanisms to obtain and control long range order from a non-conjugated bipolar block copolymer. The block copolymer self-assembles into cylinders and lamellae with their axes perpendicular to the electrode surfaces. We postulate that these nanostructures will act as conduits for charge transport to promote highly efficient OLED performance.

Program impact:
Because novel electroactive polymers and oligomers with enhanced optimized properties hold the key to the field of plastic electronics, this program focuses on the design and synthesis of novel electroactive structures with excellent electrical properties, the control of their self-assembly into ordered structures that maximize energy efficiency; the study of factors that contribute to self-ordering and ultimate device performance, and the development of methods for optimal device construction. This program is highly interactive and multidisciplinary.

Interactions:
Internal interactions: Paul Alivisatos, Nitash Balsara, Jeff Kortright, Arun Majumdar, Howard Padmore, A. Zettl
External interactions: G. Hadziioannou (Strasbourg), V. Ganesan (UT Austin), M. Thompson (USC); M McGehee (Stanford), Intel, Nanosolar.

Recognitions, Honors and Awards: ***Segalman*****:** Intel Young Faculty Seed Award. ***Frechet***: 2005 Esselen award for Chemistry at the Service of the Public; 2005 Chemical Communications Anniversary Lecture Award; National Academy of Sciences, National Academy of Engineering, American Academy of Arts and Sciences, Fellow AAAS; American Chemical Society Award in Polymer Chemistry 2000, American Chemical Society Salute to Excellence Award 2001, American Chemical Society Cope Scholar Award 2001, American Chemical Society Award in Applied Polymer Science. *Plenary Lecturer at the following 2005 Conferences*: Spanish Polymer Congress, Polymers for Africa Conference, Macro group UK, Int. Light Scattering Conference, MC7 Edinburgh RSC Materials Conference. Bayer Lecturer Univ. Massachusetts; Doctor of the University, Univ. of Ottawa, Canada 2004; Associate Editor Journal of the American Chemical Society.

Personnel Commitments for FY2005 to Nearest +/- 10%:
J. Frechet 10% (PI, program leader), R. Segalman 10% (co-PI), V. Subramanian 10% (co-PI);
L. Deng (student, 50%) F. Lauterwasser (postdoc 100%), D. Poulsen (student 50%); K. Puntambekar, (Postdoc, 100%); J. Lee, (student, 50%); B. Mattis, (student, 50%); B. Olsen (student, 50%), Y. Tao (Student, 50%), S.Y. Jang (Postdoc, 100%)

Authorized Budget (BA):
FY03 BA $493,000 FY04 BA $599,000 FY05 BA $861,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Electronic Materials Program
FWP Number: KC13

Program Scope:
The goal of the Electronic Materials Program is to advance the fundamental understanding of the materials science of semiconductors. The research focuses on the relationships between synthesis and processing conditions and the structure, properties, and stability of semiconductor materials systems. Progress in these areas is essential for the performance and reliability of a number of technologies that lie at the heart of the DOE mission including ultrahigh efficiency photovoltaic energy conversion devices, high efficiency solid-state sources of visible light, visual displays, and of a large variety of sensors and power control systems for energy generation, conservation, and distribution.

Major Program Achievements (over duration of support):
Pioneered scientific applications of isotopically controlled semiconductors; performed definitive impurity and self diffusion studies in Group IV and III-V semiconductors using stable isotope superlattices. Developed new and predictive theory (band anticrossing model) to explain properties of "highly mismatched" semiconductor alloys (HMAs) such as GaN_xAs_{1-x} and discovered new II-VI-based HMAs, including the first demonstration of a multiband semiconductor. Contributed significantly to the understanding of InN as a narrow gap semiconductor. Pioneered the use of pulsed laser melting for the synthesis of highly non-equilibrium alloys, including HMAs and "spintronic" materials. Developed fundamental understanding of the relationship between native defects and the achievable limits for semiconductor doping. Developed advanced electron microscopy methods to quantify the growth mechanisms of extended defects and to determine the atomistic core structure of dislocations in group III nitride semiconductor thin films and heterostructures.

Program Impact: Over the course of many years of sustained BES funding, the Electronic Materials Program has discovered new classes of semiconducting materials (e.g., II-VI HMAs) and has contributed significantly to the synthesis and fundamental understanding of a large number of elemental and compound semiconductors. Basic research in the Program concerning the interplay of extended defects, compositional fluctuations, and the resulting strain distributions and the light emission mechanism in GaN and InGaN aided the development of solid state lighting based on this materials system. Most recently, Program research has established that both In-rich InN and certain II-VI and III-V HMAs show promise as entirely new types of high efficiency solar cells and other opto-electronic devices.

Interactions:
Internal—National Center for Electron Microscopy, Advanced Light Source.
External—Stanford Synchrotron Radiation Laboratory, Hewlett-Packard, Agilent, MPI Stuttgart, Xerox, NREL, Cornell Univ., Purdue Univ., Univ. of Notre Dame, MIT, Harvard Univ., Münster Univ., Germany

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
J. W. Ager III – co-author, "Isotopic Effects in Solids," *Encyclopedia of Condensed Matter Physics*, co-editor, Topical Issue of *Semiconductor Science and Technology*, "Group III-N-V Alloys," 2002.
E. E. Haller – Turnbull Award, MRS, 2005; Fellow of AAAS, 2004; Recipient James C. McGroddy Prize for New Materials of the American Physical Society, 1999; Chair, 20th Intl. Conf. on Defects in Semiconductors (20th ICDS), Berkeley, CA 1999; Recipient Max-Planck Research Award, 1994; Research Professor, Miller Foundation for Basic Research in Science, 1990 and 2001; Fellow, American Physical Society, 1986; A. von Humboldt US Senior Scientist Award, 1986.
Z. Liliental-Weber – Chair, IEEE Semiconducting and Insulating Materials Conference (SIMC-X), Berkeley, CA 1998.
W. Walukiewicz – Chair, Gordon Res. Conf. on Defects in Semiconductors 2006; author, invited Topical Review, *J. Phys. D*, "Electronic Properties of InN," co-editor, Topical Issue of *Semiconductor Science and Technology*, "Group III-N-V Alloys," 2002, NTT distinguished Professorship 1990.
E. R. Weber – Fellow, American Physical Society (APS), 2001; Humboldt Senior US Scientist Award, 1994.

Personnel Commitments for FY2005 to Nearest +/- 10%:
E. E. Haller (20%), J. W. Ager III (40%), D. C. Chrzan (10%), O. D. Dubòn, Jr. (10%), Z. Liliental-Weber (50%), W. Walukiewicz (80%), E. R. Weber (10%), K. M. Yu (50%).

Authorized Budget (BA):
FY03 BA $1,262,000 FY04 BA $1,392,000 FY05 $1,348,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP title and possible subtask under FWP:
Anistropy and Chemical ordering in Vapor Deposited Amorphous and Crystalline Alloy Magnetic Films
FWP Number: KC22
Program Scope:
Vapor deposition growth is used to create new magnetic materials with structures and compositions not found in the bulk equilibrium phase diagram, including multilayers, amorphous materials, metastable alloys, and nanocrystalline materials. Perpendicular magnetic anisotropy and short or long range chemical order is created in materials by careful control of the vapor deposition process.
Major Program Achievements (over duration of support):
We have shown that perpendicular magnetic anisotropy in amorphous Tb-Fe and crystalline cubic (fcc) Co-Pt alloys (and related materials) is a growth-surface-induced effect, the result of equilibrium surface properties trapped into the growing film by low bulk diffusion. A primary characteristic feature of this growth-surface induced anisotropy we showed is that the magnetic anisotropy is independent of film thickness and strain, and is enhanced by increasing surface mobility (primarily by increasing the growth temperature up to the point of the onset of significant bulk diffusion, but also by reducing deposition rate or decreasing surface roughness), but vanishes upon annealing, all without obvious changes in the structure of the material. In amorphous Tb-Fe alloys, we suggested (through modeling) that the anisotropy is due to effects much like the well-known texturing of vapor-deposited polycrystalline materials. In epitaxial (100), (110), (111) and polycrystalline films of $CoPt_3$ and related fcc-like Co-Pt and Ni-Pt alloys: (1) we showed that the anisotropy is related to a clustering of Co into planar platelets at the growth surface, despite the significant negative energy of mixing for Co-Pt (meaning chemical ordering (mixing) not clustering is favored); and (2) that this is due to Co segregation to step edges, which cause Co platelets to form as the islands coalesce.
Program impact:
We have shown that perpendicular magnetic anisotropy in films does not require an intrinsically axially symmetric structure such as a multilayer or hexagonal close packed structure, but can instead be easily produced by the intrinsic asymmetry of the vapor deposition growth process in a material. This includes in particular materials such as amorphous or cubic crystalline materials which seem a priori to not allow the uniaxial symmetry breaking of perpendicular anisotropy. Step edge segregation is a phenomenon which is likely to occur in a broad range of materials and will lead to asymmetric properties in many materials which have not yet been observed because they were not expected.
Interactions:
David Smith, Arizona State University;
Matt Carey, Hitachi San Jose;
V. G. Harris, Northeastern; Julie Cross, University of Washington; M. Newville, University of Chicago;
D. Haskel and J. Freeland, Argonne National Lab
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Kathryn McCarthy Lectureship (2004)
APS-Keithley Instrumentation Award (2006)
Personnel Commitments for FY2005 to Nearest +/- 10%: (provide name where relevant):
F. Hellman, PI
Daniel Queen GSR (20%)
David Cooke GSR (50%)
Zoe Boekellheide GSR(100%)
Mark Wong: GSR (stipend and tuition support by physics dept fellowship) (100%)
Erik Helgren - assistant project scientist (33%)
Authorized Budget (BA):
new project: FY05 BA $155,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP title and possible subtask under FWP:
Energetics of Nanomaterials
FWP Number: KC22
Program Scope:
Thermodynamic properties of nanostructured materials, specifically studying how energy, entropy, and heat capacity depend on particle size A particular focus is on the thermodynamic comparison between bulk nanoparticle systems and vapor-deposited nanocrystalline and multilayer films.
Major Program Achievements (over duration of support):
In materials which are nanoscale, whether a nanocomposite or a granular film, or a multilayer, virtually all properties are affected by the presence of the surfaces and the finite size of the particles or layers. The effects include those which one might call intrinsic, e.g. suppression of a magnetic ordering temperature due to fluctuations and reduced coordination of surface atoms or quantization of electronic states, and those which one might call extrinsic or at least more materials-related, such as surface reconstruction and segregation of one element to the surface of the particle, or water absorption on the surfaces, or strain from an epitaxial relationship with a second component such as in a multilayer or granular material. We have studied the Neel temperature for thin CoO in various types of multilayered and nanocrystalline materials, and have demonstrated both types of effects.
Program impact:
We have shown that Neel temperature suppression in CoO can be due to either true finite size effects (the two-dimensional nature of a thin film) or due to either the crystallographic disorder produced by the interactions with the substrate or other underlying layer or effects such as water absorption at grain boundaries. We have also shown that the finite grain size of a nanocrystalline film produces a generic phonon softening which increases the entropic stabilization of nanocrystalline structures.
Interactions:
Alexandra Navortsky, UCDavis;
Brian Woodfield and Julie Boerio-Goates, BYU;
Nancy Ross, VTU
Ami Berkowitz, UCSD
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Katheryn McCarthy Lectureship (2004)
APS-Keithley Instrumentation Award (2006) (this DOE grant provided primary support for this work)
Personnel Commitments for FY2005 to Nearest +/- 10%: (provide name where relevant):
F. Hellman, PI
Daniel Queen GSR (80% of his time)
David Cooke GSR (50%)
Authorized Budget (BA):
new project **FY05 BA $**75,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020201

FWP title and possible subtask under FWP:
H- Production Research

FWP Number: KC21

Program Scope:
Development of a new negative hydrogen (H-) ion source configuration that combines a standard multicusp H- source chamber (as currently used in the Spallation Neutron Source front end) with a microwave-driven ECR ion source chamber. By using the ECR plasma as a driver, this method eliminates the fragile internal RF antenna that is frequently used in today's H- volume production sources. Our goal is to demonstrate high beam current density and long life operation. As part of this project, we will also design a new negative ion extraction geometry that makes use of a novel electron dumping and beam steering system.

Major Program Achievements (over duration of support):
The apparatus was designed and constructed. In testing the ECR source alone, we had extracted up to 1.5 A of electrons. After some modifications, the experiment using the new configuration was able to ignite a pulsed discharge of 17.5 A, with a pulse length of 2 ms at 30 Hz. However, the negative ion current was found to be low, in agreement with a correspondingly low plasma density in front of the extraction aperture. We are trying new ways to improve the performance.

Computer simulation of the new ion extraction geometry has produced a design that met the requirements.

Program impact:
If successful, an advanced H- ion source can be used to upgrade the Spallation Neutron Source (SNS), and significantly increase the beam current and neutron yield at the target. It can also be used for future "proton driver" accelerators.

Interactions:
Ion source & injector group at the Spallation Neutron Source (SNS), Oakridge, TN

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

Personnel Commitments for FY2005 to Nearest +/- 10%: (provide name where relevant)
Rod Keller (principal investigator) 50% before July 1, 2005
Joe Kwan (principal investigator) 50% after July 1, 2005

Authorized Budget (BA):
FY03 BA $ **FY04 BA $300,000** **FY05 BA $300,000**

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Resonant Soft X-Ray Studies from Hard and Soft Nanostructured Matter
FWP Number: KC22

Program Scope:
We combine unique sensitivity of core-resonant soft x-ray spectroscopies with angle-resolved scattering to gain fundamental insight into functional heterogeneity in emerging hard and soft materials. Our initial focus was on magnetic materials, where we continue to develop and apply resonant scattering measurements that can sense lateral and depth variations of chemical and magnetic properties with nanometer spatial resolution. Of increasing interest are soft condensed systems, where resonant scattering effects at the carbon, nitrogen, and oxygen edges yield unique contrast mechanisms to study heterogeneity in polymers and other organic systems.

Major Program Achievements (over duration of support):
Developed unique endstation for soft x-ray magneto-optical studies in fields up to 1.5 Tesla and vs. temperature. Developed standing wave and specular reflectivity techniques to depth resolve magnetic and chemical variations across buried interfaces. Developed resonant small-angle scattering techniques to study magnetic and chemical heterogeneity and applied them in a variety of granular alloy, multilayer, and nanoparticle systems having both in-plane and perpendicular anisotropy. Extended partially coherent scattering techniques into the coherent scattering (magnetic speckle) regime. Developed polarization-resolved x-ray magneto-optical Kerr effect measurements and applied them to resolve depth-dependent magnetization changes in exchange-spring and exchange-bias structures. Extended core-resonant scattering techniques for studies of heterogeneous polymer systems at the carbon K edge.

Program impact:
The general applicability of resonant soft x-ray scattering to study chemical and functional heterogeneity is attracting researchers from hard and soft matter communities to DOE synchrotron radiation facilities. Unique resonant contrast mechanisms complement hard x-ray and neutron scattering approaches, and are beginning to impact our understanding of structural aspects of diverse systems that are difficult to understand with other techniques. Development of experimental capabilities and rigorous analytical techniques attract collaborators from industry, national labs, and universities to form a growing program at the ALS to apply these techniques to a broad range of systems of both fundamental and technological interest. Direct sensitivity to chemical and functional properties down to nanometer length scales in small sample volumes will make these techniques increasingly relevant to emerging nanoscale materials.

Interactions:
Hitachi Global Storage Technology (E.E. Fullerton); LBNL (C. F. Fadley, Center for X-Ray Optics, ALS); Argonne National Lab (S.D. Bader); UC Berkeley (Y. Suzuki, F. Hellman, R. Ramesh, R. Segalman, N. Balsara); UC San Diego (S. Sinha, I.K. Schuller); U. Oregon (S. D. Kevan); U. Washington (L. Sorenson); U. Colorado (D. Dessau): Ohio State University (A. Epstein), Dow Chemical (G. Mitchell); Los Alamos National Lab (M. Fitzsimmons, R. Hjelm); U. North Carolina (H. Ade)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
19 invited talks or University colloquia since 2000.

Personnel Commitments for FY2005 to Nearest +/- 10%:
J. B. Kortright (PI) 100%

Authorized Budget (BA):
FY03 BA $180,000 FY04 BA $205,000 FY05 BA $180,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Bridging the Gap between Electronic, Spin, and Lattice Degrees of Freedom in Novel Complex Materials Research
FWP Number: KC22
Program Scope:
Our research program focuses on the study of novel materials, beyond the Fermi liquid paradigm, characterized by the emergence of new forms of orders and exotic phases. Potential applications of these materials are in the area of energy and hydrogen storage. Examples of these materials are strongly correlated materials and carbon based materials. Additionally we are also developing a novel instrumentation to investigate the magnetic properties of spintronics materials.
Major Program Achievements (over duration of support):
1) Isotope dependent study of high temperature superconductors: We have continued our effort to study the effect of the lattice on the electronic properties of cuprate with emphasis on the tendency to charge ordering. We have shown that the electron lattice interaction (Phys Rev Lett. 2005) is strong and that it enhances the tendency of the system toward charge ordering (Submitted Phys. Rev. Lett. 2005). This work has received a several instances of media coverage in print and television. Our main focus in the field of carbon-based materials has been so far in graphite and synthesis of graphene.
2) Carbon-based materials: In the study of graphite we have provided the first direct experimental evidence of how the interlayer coupling modifies its band structure with respect to the case of a single graphene layer, and provided the first evidence of two types of charge carriers (electrons and holes) in graphite. Although this has been known theoretically for more than 40 years, our work (Phys. Rev. Lett. 2005) constitutes the first direct experimental proof. Our work on polycrystalline graphite (Phys. Rev. B-Rapid Comm. 2005), has put forward a new proposition in the field of photoemission: the possibility of studying the momentum resolved band structure of polycrystalline materials, something previously believed to be impossible. This has the potential to extend this probe to a huge class of materials where single crystals cannot be produced. We have also developed a synthesis effort focusing on the growth of single and double layer graphene to study the evolution of the electronic properties in the transition from a purely two dimensional system to a three dimensional system.
3) Development of a spin polarized analyzer: In the past year we have performed the first testing of the analyzer with a single drifting tube. The test will now be extended to the final setup with three tubes. The systems is expected to be functional by next march.
Program impact:
The impact of the following research activity will provide a unique tool to understand the unconventional role of the lattice and the relevant scattering processes in strongly correlated materials as high temperature superconductors. On the other hand the development of a new Spin detector will enable the investigation of a wider range of materials as half metals, spintronics materials, etc. and will allow a direct mapping of the spin degrees of freedom, recognized fundamental for the properties of many novel phenomena.
Interactions:
Internal — Advanced Light Source (ALS); National Center for Electron Microscopy; Material Science Division; Department of Physics, University of California Berkeley.
External — University of Tokyo, Japan; Electrotechnical Laboratory (ETL), Tsukuba-Japan; University Pierre et Marie Curie, Paris- France; Polytechnic of Milano - Italy; Georgia Institute of Technology, USA.
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Outstanding Performance Award, Lawrence Berkeley National Laboratory (2005);
27 Invited talks and Invited Seminars between October 2004 - October 2005
23 instances of media coverage to my work in print and on television, including a documentary on Italian National TV (Rai 3) broadcast during prime time in Italy and other European Countries.
Co-organizer of the Annual Meeting: Physics by the Bay - IV Edition - Berkeley 2005
Personnel Commitments for FY2005 to Nearest +/-10%:
Alessandra Lanzara (PI) 80%; Gey-Hong Gweon (Associate Researcher) 100%, Kyle McElroy (Post-doc) 100%, Jeff Graff (Visiting researcher) 100%, Shuyun Zhou (PhD Student) 80%, Chris Jozwiak (PhD Student) 80%, Elizabeth Rollings (Researcher) 100%.
Authorized Budget (BA):
FY03 BA $ 150,000 FY04 BA $ 428,000 FY05 BA $ 428,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020203

FWP and possible subtask under FWP: Theoretical study of strongly correlated materials
FWP Number: KC23

Program Scope:

Establish the theoretical framework for understanding doped Mott insulators. Specific projects are as follows. 1) Understand why do all known Mott insulators break symmetry. Provide theoretical guidance for the search of featureless Mott insulators. 2) Understand the interplay between spin, charge and lattice excitations in high T_c superconductors. 3) Understand the disparity between the properties of nodal and antinodal quasiparticles in the cuprates.

Major Program Achievements (over duration of support):

During the period of 2004-2005 the PI has published 15 journal articles. Among them are 2 **Nature**, 2 **Science**, 6 **Physical Review letter** papers. In the following we selected some highlight from the above results.

1) The P.I.'s group found a new conservation law that can protect a Mott insulator from developing symmetry breaking. This new conservation law unifies the two primary novel quantum liquid discovered in the past twenty years: the fractional quantum Hall liquid and the quantum dimmer liquid. It also suggest a new direction for the search of new exotic states of matter. (Los Alomos eprint # cond-mat/0509071, accepted by Physical Review letter).
2) The quasiparticles interference model for high Tc superconductor continues to receive experimental interest and supports. We (P.I. and Seamus Davis's group) achieved in identifying the origin of the quasiparticles scattering in $Bi_2Sr_2CaCu_2O_{8+x}$ (*Science* **309**: 1048, 2005). We (PI and Lanzara's group) have confirmed the quasiparticles interference model by directly compare the autocorrelation function of the ARPES study with the Fourier transform STM studies. (Los Alomos eprint # cond-mat/0505333, accepted by Physical Review letter).
3) We (P.I. and Lanzara's group) identified the significant different coupling strength between phonons and the nodal/ antinodal quasiparticles. (Nature **430**, 187 (2004). The PI's group and C. Honerkamp of the Max Planck Institute have performed a renormalization group calculation to elucidate the interplay between charge, spin and lattice degrees of freedom in the cuprates. (Los Alomos eprint # cond-mat/0509072, submitted to Physical Review Letters.)

Program Impact:

1. The condensed matter community has been searching for featureless Mott insulator in the past fifteen years. The traditional guideline in this search is "frustration". Recently the PI's group found a new conservation law that can protect a Mott insulator from developing symmetry breaking. This work may open a new direction in the longstanding effort in searching for "featureless Mott insulators".

2. The prediction and observation of quasiparticle interference in the $Bi_2Sr_2CaCu_2O_{8+x}$ high temperature superconductors is widely regarded as a highlight in the field of high T_c superconductivity in recent years. In the long run, the lasting impacts of this work lie in the fact that it shows low-energy nodal quasiparticles are well defined while the antinodal quasiparticles are incoherent. This mysterious nodal-antinodal dichotomy is a novel manifestation of how the spin, charge, and lattice excitations couple to electron quasiparticles.

3. The ``dichotomy'' between nodal and antinodal quasiparticles pointed out in the collaboration with the Shen's group has become a central issue of high T_c superconductivity.

Interactions:

University of California, Berkeley, Cornell University, Stanford University, Advanced light source

Recognitions, Honors and Awards (at least in some part attributable to support under this program):NA
Personnel Commitments for FY2003 to Nearest +/- 10%:

Dung-Hai Lee (PI), summer
Alex Seidel (postdoc) 100%
Henry Fu (student) 50%

Authorized Budget (BA):

FY03 BA $81,000 FY04 BA $81,000 FY05 BA $81,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Microscopy Investigations of Quantum Dots, Nanorods, and Soft Condensed Matter
FWP Number: KC31

Program Scope:
This program aims to stretch the limits in the state-of-the-art of optical characterization, through the development of novel forms of optical microscopies, such as single pulse CARS microscopy with phase control, apertureless NSOM (ANSOM), and femtosecond pump-optical injection probing spectroscopies of single nanostructure species under stimulated emission conditions. A parallel molecular beam epitaxy growth effort for processing semiconductor materials with in situ scanning tunneling microscopy is used to study the growth mechanisms of III-V nitrides. Development of novel microscopies provide new spectral and spatial windows into the analysis of materials for DOE missions in energy utilization.

Major Program Achievements (over duration of support):
Growth studies of flat GaN and InN, as well as islands of InN and InGaN have been performed in an apparatus that incorporates scanning tunneling microscopy with molecular beam epitaxy. Growth mechanisms of GaN have been analyzed by tunneling microscopy images. Apertureless near field microscopy studies of GaN and InN islands have revealed contrast mechanisms due to the real and imaginary parts of the index of refraction, measuring nanometer size Ga metal islands, and probing InGaN islands. Pickup of gold nanoparticles permits tip enhancements with resolution of the electric field phase in the images. Ultrafast laser, differential gain experiments on ZnO lasing in nanowires and tetrapods have been performed to measure the timescales and ratios of electron-hole plasma and exciton mechanisms during lasing in nanostructured materials. Two novel types of measurements have been performed, stimulated emission dumping and upconversion probing methods. A single pulse CARS microscopy project using an ultrafast laser and phase control with interferometric detection produces complete Raman spectra while spatially scanning. Polymer domains have been analyzed with vibrational spectral sensitivity.

Program Impact:
New forms of microscopy with chemical specificity have significant impact on the semiconductor industry, related to the study of patterning, line dimension reduction, nanostructure lasers, and materials analysis. Studies of InGaN are important for the lighting industry and for energy efficiency.

Interactions:
A collaboration with IBM scientists, William Hinsberg and Frances Houle to advance the state of the art in detection of latent images in lithographic polymer films.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Invited Speaker at American Chemical Society Nobel Laureate Signature Symposium on Nanoscience
2005 Peter Debye Prize, American Chemical Society

Personnel Commitments for FY2004 to Nearest +/- 10%:
S. **Leone** (PI) 5%
B. Liu (postdoc) 50%
D. Chen (postdoc) 80%
J. Szarko (graduate student) 40%
J.-K. Song (postdoc) 75%
A. Caster (graduate student) 25%
S.-H. Lim (postdoc) 10%
Olivier Nicolet (postdoc) 10%
Larissa Stebounova (postdoc) 80%

Authorized Budget (BA):
FY03 BA $389,000 FY04 BA $390,000 FY05 $390,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP title and possible subtask under FWP: Mechanics, Dynamics and Transport in Assemblies of Soft-Hard Nanomaterials
FWP Number: KC12

Program Scope: The overall program goal is to advance the fundamental understanding of complex phenomena in soft and hard nanomaterials. The research focuses on two areas: (i) understanding of transport of liquids, ions, and biomolecules in ***nanofluidic*** channels: This explores a new class of nanomaterials to study molecular and ionic transport in confined or low-dimensional liquids. (ii) investigating a new class of biomimetic molecules called ***peptoids***, which have the same backbone structure as peptides but with a residue diversity of ~ 1000. The scope is to explore the ability of sequence-specific peptoids to recognize non-biological molecules.

Major Program Achievements (over duration of support):

- Used ionic confinement in fluidic nanotubes and nanochannels and demonstrated ion selection and unipolar solutions
- Showed that the ionic conductance in nanochannels is about 10^4-10^5 times higher than predicted by bulk theory.
- Created the first nanofluidic transistor and demonstrated transconductance
- Demonstrated an interesting ionic transition during DNA translocation and protein reaction influidic nanotubes/nanochannels and showed that it can be used to measure the charge-to-volume ratio of biomolecules
- Developed micro-cantilever and micro-membrane arrays for studying nanomechanics of molecular reactions in high-throughput manner.
- Demonstrated mechanical reactions of kinase reactions in real-time
- Developed surface chemistry protocols for attachment of biomolecules and preventing biomolecules from nonspecific binding

Program impact: The impact of studying aqueous solutions of ions and biomolecules could have significant impact on fundamental understanding of water, with implications in water purification, biochemical assays at possibly single cell levels, and electrochemical energy conversion/storage. The study of peptoids as a class of sequence-specific biomimetic molecules could have significant impact on our fundamental understanding of various molecular processes such as recognition, catalysis, energy conversion (e.g. photoluminescence) etc.

Interactions:
Peidong Yang (Dept. of Chemistry, UCB and MSD, LBL); Arup Chakraborty (Depts. of Chem. Engr & Chemistry, UCB and MSD, LBL); Frank Chen (Life Sciences Division, LBL); Ron Zuckermann (Chiron Corp.).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
(i) Elected to National Academy of Engineering; (ii) Member, Nanotechnology Advisory Group, President's Council of Advisors on Sci. & Tech. (PCAST); (iii) Midwest Mechanics Lectureship; (iv) Invited Lecture – Frontiers in Mechanical Engineering, U Penn; (iv) 15 Academic Invited Talks; 12 Conference Invited Talks; 3 Industry Invited talks.

Personnel Commitments for FY2005 to Nearest +/- 10%: (provide name where relevant)
Arun Majumdar (PI): 10 %
2 Graduate Student: 49.5% 9 month academic year + 100 % 3 month summer (one working on nanofluidics and the other working on peptoids)
1 Post-doc fellow: 100 % 4 months.

Authorized Budget (BA):
FY03 BA $162,000 FY04 BA $230,000 FY05 BA $230,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Time-resolved optical spectroscopy of correlated electron systems
FWP Number: KC22

Program Scope:
Development of advanced techniques of time-resolved optical spectroscopy and application to systems of correlated electrons. High-precision time-domain spectroscopy exploring the linear and nonlinear response of superconductors in the terahertz frequency domain. Heterodyne detection of transient grating allowing direct real-space observation of the propagation of quasiparticles in correlated electron metals. Direct measurement of electron spin diffusion using transient spin gratings. Contactless measurement of conductance of oxide heterostructures by time-domain terahertz spectroscopy.

Major Program Achievements (over duration of support):
Pioneeered research in terahertz optical conductivity of the vortex state of high-Tc superconductors. First observation of the optical Hall conductivity of both quasiparticles and vortices.

Direct measurement of the rate of phase fluctuations of the superconducting order parameter in a high-Tc superconductor. Demonstration that phase transition from superconducting to normal state is driven by phase fluctuations. Proof of absence of superconducting fluctuations in the pseudogap regime.

First measurement of the quasiparticle scattering rate in the high-Tc superconductor BSCCO by optical conductivity measurements. Identification and theoretical explanation of a component of the optical conductivity originating from extreme heterogeneity of the local superfluid density.

First direct observation of quasiparticle propagation in a high-Tc superconductor, using heterodyne transient grating spectroscopy. Time-resolved detection of quasiparticle motion lead to direct measurement of the quasiparticle diffusivity tensor, inelastic, and elastic scattering rates in high-quality YBCO and BSCCO single crystals.

First measurements of the spin diffusion coefficient of a two-dimensional electron gas and observation of theoretically predicted spin-Coulomb drag effect.

Program impact:
Recognized internationally as leading group using advanced laser-based techniques to discover effects and obtain data not available using conventional spectroscopic methods.

Interactions:
Stanford University (Prof. S. Zhang)
UC Santa Barbara (Prof. David Awschalom)
CRIEPI, Japan (Dr. Yoichi Ando)
University of British Columbia (Profs. W.N. Hardy and D.A. Bonn)

Recognitions, Honors and Awards
Chair, Gordon Conference on Correlated Electron System (2002-present)
Vice-chair, Gordon Conference on Correlated Electron Systems (2002)
Chosen by editors of Science to write review of advances in the physics of high-Tc superconductors
International and national invited talks, including APS March Meeting, Aspen Center for Physics, Institute for Theoretical Physics (Santa Barbara), International Center of Physics (Trieste), Gordon Conference on Superconductivity (Oxford, UK), and Symposium on SPC Coupled Materials (Tokyo).

Personnel Commitments for FY2003 to Nearest +/- 10%: J. **Orenstein** (group leader) 30%,
Matthew Langer (grad student) 100%
Colleen Kantner (grad student) 50 %
Authorized Budget (BA):
FY03 BA $184,000 FY04 BA $ 184,000 FY05 BA $184,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Low-Temperature Properties of Materials
FWP Number: KC31

Program Scope:
Specific-heat measurements, including measurements under pressure and in magnetic fields, are used to investigate relations between chemical composition, structure, and physical properties. Areas of emphasis include: unusual superconductors for which specific-heat data give information about the underlying electronic properties and the mechanism of the electron pairing; the relation between magnetism and superconductivity in heavy-fermion compounds; the use of small-sample techniques to study materials available only in small quantities.

Major Program Achievements (over duration of support):
Improved instrumentation for small-sample relaxation calorimetry has been developed and tested in the 1 – 25 K region. Ambient-pressure specific-heat and thermal-expansion measurements on UGe_2 have shown the existence of a transition in the vicinity of 25 K, which is related to the occurrence of superconductivity at 12 kbar. The specific heat of three samples of the recently discovered novel superconductor $Na_{0.3}CoO_2$ 1.3 H_2O have been reinterpreted in the light of recent information on changes that take place in this material with ageing of the samples.

Program impact:
The measurements on UGe_2 have established the ambient-pressure intercept of the phase boundary for the transition that is associated with the occurrence of superconductivity at the 0-K quantum critical point at 12 kbar, and will give information about the transition, which is of interest in connection with the nature of the QCP and the superconductivity. The phase boundary itself had not been well established in the low-pressure region, and the nature of the transition has also not been well characterized. In combination with recent information on other ageing effects on the properties of $Na_{0.3}CoO_2$ 1.3 H_2O, the specific-heat data have shown the extreme sensitivity of the electronic structure and the superconductivity to the presence of O vacancies. The results show the evolution of these properties with increasing concentration of vacancies, culminating in a charge-ordered state that does not support superconductivity. The improvements in instrumentation for relaxation calorimetry will support future measurements on nanoparticles and carbon nanotubes.

Interactions:
Internal: P. Alivisatos; A. Zettl; M. Cohen; S. Louie. External: LLNL, LANL; Centre Etude Nucleaire Grenoble; Amherst College; Princeton University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask: Invited talks: Osaka-Grenoble Summer School on Heavy Fermion Matter, CNRS, Grenoble, France, July 2005.

Personnel Commitments for FY2005 to Nearest +/- 10%:
N. E. **Phillips**, 75% on project, paid ~5%; R. A. Fisher, ~25% on project, paid ~5%; Fred Hardy, 100% on project, paid 100%;Yee Wong, ~10 %.

Authorized Budget (BA):
FY03 BA $151,000 FY04 BA $151,000 FY05 $150,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Nuclear Magnetic Resonance
FWP Number: KC31
Program Scope: The nuclear magnetic resonance (NMR) program has two complementary components. The first is the establishment of new concepts and techniques in NMR and its offspring, magnetic resonance imaging (MRI), in order to extend their applicability and enhance their capability to investigate molecular structure and organization from materials to organisms. The study and diagnostic use of nuclear spins interacting with each other and with others degrees of freedom requires the development of new theoretical and experimental methods; one consequence of these efforts is the design and fabrication of next-generation NMR and MRI equipment. The second component of the research program involves the application of such novel methods, together with other programs, and with outside laboratories and industry, to significant problems in chemistry, materials science, and biomedicine. It is the unique environment of interdisciplinary research and large-scale instrumentation capabilities at the Lawrence Berkeley National Laboratory that cultivates these innovations, their diverse applications, and technology transfer.

Major Program Achievements (over duration of support): Some principal developments: Helped launch high-resolution solid-state now widely used in materials, chemistry and biology; introduced multiple-quantum spectroscopy; developed zero-field Fourier-transform NMR using both field cycling and superconducting detectors; introduced dynamic-angle spinning and double rotation for quadrupolar nuclei such as oxygen-17 and aluminum-27; made advances in optically pumped and detected NMR and MRI, and the development of novel xenon-based NMR molecular sensors; most recently, introduced ex-situ scanning, remote detection, and ultralow and zero-field SQUID and laser magnetometer detection of NMR and MRI, opening the way to in-the-field observation of objects and subjects not amenable to normal methods of NMR and MRI. Examples of applications: flow and dispersion of fluids in porous materials, and recent development of microfluidic NMR and MRI "on a chip," studies of structure and dynamics in minerals and oil reserves, catalysts, semiconductors, surfaces, amorphous materials, nanocrystals, nanotubes, polymers, biomolecules, tissue, organisms, diagnostic biomedical molecular imaging.

Program impact: "Seeing is believing"; novel techniques and devices of magnetic resonance spectroscopy and imaging have expanded our ability to "see" into materials and organisms. The concepts and instrumentation, adopted worldwide by laboratories and industry, are being used to investigate molecular structure and organization from the nanoscale dimensions of catalysts and polymers to the macroscopic proportions of human imaging and oil exploration. Education: hundreds of scientists ("Pinenuts") trained in the laboratory, many holding leading positions in academia and industry. Patents: more than twenty issued, filed, pending or disclosed methodologies licensed, adapted into commercial NMR technology. Journal Covers: eg Science, Spectroscopy, J. Mag. Resonance, Angewandte Chemie, J. Physical Chemistry. Press Articles: e.g. C&E News, Science, Nature "News and Views", Science News, Scientific American, Biophotonics, Analytical Chemistry, R&D Magazine.

Current Interactions: J. Reimer (EEHS and Chemical Engineering), D. Wemmer (Physical Biosciences and Chemistry), J. Clarke (MSD and Physics), D. Budker (NSD and Physics), T. Budinger and S. Conolly (LSD and Bioengineering), S. Prusiner and M. Shuman (UCSF). Industry: eg Schlumberger-Doll Research, GE, Varian.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): e.g. Glenn T. Seaborg Chair, UC Berkeley; Docteur Honoris Causa Universities of Rome and Paris: Member, National Academy of Sciences; DOE E.O. Lawrence Award; Wolf Prize in Chemistry; Centenary Medal, Royal Society of Chemistry; ACS Irving Langmuir Award; ACS F.A.Cotton Medal; Tetelman Fellow, Yale U; Ampere Congress Honoring AP's 50'th Birthday; R&D-100 Awards; Univ Calif Distinguished Teacher Award; Professeur Joliot-Curie; Ecole Superieure Phys Chem, Paris; Loeb Lecturer, Harvard U; Lord Lecturer, MIT; Roberts Lecturer, Caltech; Hinshelwood Professor, Oxford U; Lord Todd Professor, Cambridge U; Faraday Medal Royal Society; Seaborg Medal UCLA; Scientific American "50 Visionaries;" Elected Foreign Member, Royal Society (London): 60th Birthday International Ampere Symposium in Honor of Alex Pines, Chamonix France (2005); Distinguished Visiting Professor e.g. Singapore, Taipei, Paris, Weizmann, etc (2005): Medal of the NMR Society of Japan (2005).
Web Pages: http://waugh.cchem.berkeley.edu/research/ http://waugh.cchem.berkeley.edu/alex/

Personnel Commitments for FY2005: A. **Pines** PI 25%, 15 graduate students, 6 postdoctoral fellows.

Authorized Budget (BA):
FY03 BA $899,00 FY04 BA $872,000 FY05 BA $872,000

Laboratory Name: Lawrence Berkeley Nat. Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP:
Materials Sciences Division: Properties of Ceramics and Interfaces Program

FWP Number: KC13

Program Scope:
A multidisciplinary investigation of interface composition, structure/bonding and mechanical properties provides new comprehension of atomic level structure that can motivate development of superior ceramics and related interfacial structures. Specifically, ceramic grain boundaries and dissimilar interfaces are evaluated and results related to interface-dictated properties, including mechanical and thermo-chemical stability, kinetic and dynamic behavior.

Major Program Achievements (over duration of support):
A set of *in situ* toughened ceramics, ABC-SiC, with excellent toughness, creep, wear and fatigue strength to 1400°C was developed. Corollary results include: elucidated how additives dictate derived grain morphology and character of the nanoscale intergranular films (IGFS), that are critical to achieving superior cold to hot behavior in SiC and Si_3N_4; correlated properties with atomistic computations and continuum modeling of IGF structure, stability and properties; assessed the atomic location and bonding of additives in Si_3N_4 IGFs via STEM imaging; and determined important, but rarely known worst-case cracking thresholds, intrinsic toughnesses and short crack R-curves for several ceramics.

Developments in processing include: 1) Cu wire-Al_2O_3 nanocomposites via electrochemical infiltration techniques, and 2) several novel, transient-liquid phase-based methods for joining structural ceramics that exploit multilayer, microdesigned interlayers, e.g., for joining Al_2O_3 assemblies via a dewetting liquid-film using Cu/Nb/Cu.

Interface chemistry and structure was directly related to strength, toughness and fatigue resistance of several Al_2O_3/ metal multilayers involving both model systems and Al_2O_3/(M-Al) alloy interfaces from high-temperature oxidation. The latter entails void formation, oxide layer growth processes and adherence. In these, the S interface adsorption character and adherence depend strongly on alloy content, e.g., even involving new S-Cr multilayer structures.

A suite of signature model experiments were implemented to assess the energetics of ceramic surfaces and influences of surface anisotropy on morphological evolution. Also unexpectedly strong $p(O_2)$ dependencies of surface, interface, and ceramic grain-boundary energies and kinetics for liquid metal-oxide systems were established. A hierarchy of controlling mechanisms for reactive spreading of liquids were identified and illustrated including: new model derived for ridge-limited liquid spreading at high temperature, atomic mechanisms controlling rapid liquid-metal spreading prior to ridging, and identification of surface-tension driven (Marangoni) films in metal-metal systems.

Program Impact: While developing a tunable family of SiC-based ceramics with unparalleled low-temperature strength/toughness plus hot creep/fatigue properties, new strategies were established for material optimization—exploiting *reversible changes in interface structure* via heat treatment and novel methods to assess key mechanical properties, including a new concept, the *fatigue threshold R-curve*. Guidance follows from a broad framework developed to describe interface adsorption that combines classical and new, often multilayer regimes, e.g., adsorption-induced boundary structure transitions. Paradigmatic examples include surface amorphous films on Bi_2O_3-doped ZnO. Both very strong and subtle relations of interface chemistry and toughness were exceptionally well illustrated. Hitherto unknown multiple segregation regimes at dynamic Al_2O_3/alloy interfaces were related to alloy composition and oxide phase. Radical re-evaluation of the classic Young-Dupré equation for contact angle/wetting behavior of high temperature liquids plus novel mechanistic analysis yields a breakthrough in conceiving liquid spreading at high temperatures. How anisotropy in surface evolution can profoundly influence nanostructure stability was explicated.

Interactions:
Internal—National Center for Electron Microscopy, Advanced Light Source.
External—ORNL; LLNL; SNL; ANL; LANL; IEENL; NIST; MIT; CMU; Crystal Systems Inc.; MPI Stuttgart.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
A. M. Glaeser - JSPS Invitation Fellowship, Roland B. Snow Award (American Ceramic Society)
R.O. Ritchie – Nadai Medal (ASME); Fellow of TMS; Fellow of the Institute of Physics, UK.

Personnel Commitments for FY2005 to Nearest +/- 10%:
R. O. Ritchie (10%), R. M. Cannon (50%), L. C. DeJonghe (10%), A. M. Glaeser (15%), P. Y. Hou (50%), E. Saiz (50%), A. P. Tomsia (20%), X.-F. Zhang (60%)

Authorized Budget (BA):
FY03 BA $1,321,000 FY04 BA $1,321,000 FY05 BA $1,314,000

Laboratory Name: Lawrence Berkeley
B&R Code: KC020202

FWP: Studies of the Metal/Solution Interface
FWP Number: KC22

Program Scope:
Research is conducted to determine the structure and bonding at the metal/solution interface. Surface x-ray scattering (SXS) is used to obtain a complete structural characterization of the interfacial region *in-situ* including both ions in the double layer and metal atoms at the surface. Infrared reflection absorption vibrational spectroscopy (IRRAS) is used to complement SXS for the study of interfacial species that are weakly scattering and/or lacking in long-range order, and to obtain more specific chemical bonding information. Topics under study include potential-dependent metal surface reconstruction/relaxation phenomena, the structure of discharged or partially discharged ions and the adsorption sites/geometries of neutral molecules adsorbed on the metal surface .

Major Program Achievements (over duration of support):
Developed new *in-situ* methodologies for structure determination at the metal/solution interface. Elucidation of structural phenomena at electrified interfaces that are especially interesting with respect to current theory. Potential driven reconstruction of Au(hkl) surfaces in solution shown to be related to charge at the surface and accounted for theoretically using a "gluon" Hamiltonian. The orientation of acetonile molecules in the electrical double-layer was shown to be a function of water content, nature of the cation, and the surface charge as predicted by the classical Watts-Tobin theory. Chloride and bromide ions shown to act as "surfactants" in the electrodeposition of Cu. Defects in Pt(hkl) surfaces shown to be responsible for nucleation of OH_{ad} and for the oxidation of CO at low overpotentials. Sn atoms in the surface of $Pt_3Sn(111)$ shown to be stable at potentials up to 1 V above the corrosion potential of Sn due to intermetallic bonding.

Program impact:
Methodology developed in our group for in-situ SXS at the metal/solution interface being adopted by numerous groups around the world. Improved understanding of the role of chloride ion in Cu electrodeposition used by IBM to improve the model of superfilling in on-chip metallization. Improved understanding of the corrosion resistance of alloys with strong intermetallic bonding.

Interactions:
University of Liverpool (Prof. Chris Lucas) SXS
John Dukovic (Applied Materials) electrodeposition
Panos Andricacos (IBM) electrodeposition

Recognitions, Honors and Awards (at least partly attributable to support under this FWP):
Plenary Lecture by Philip Ross at 55th International Society of Electrochemistry Meeting, Thessaloniki, Greece, September 22, 2004; Invited Lectures by Nenad Markovic at 4th International Symposium on Electrocatalysis, From Theory to Industrial Applications, 2002 Lake Como, Italy ; Workshop on Theory of Catalytic and Electrocatalytic Reactions, Hostercombe Denmark, June 15-18 (2003)

Personnel Commitments for FY2004 to Nearest +/- 10%: Philip Ross (P.I.) 20 %; Nenad Markovic 33 %, Keng Chou, 50 %

Authorized Budget (BA):
FY03 BA $156,000 FY04 BA $156,000 FY05 $156,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP: Electrode Surface Processing
FWP Number: KC22

Program Scope:
Electrocatalysts with unique properties are created by bringing two or more different metals together as small (1 – 10 nm) bi- or multi-metallic clusters dispersed on an electronically conductive support. Various synthesis methodologies are being developed to create bi- or multi-metallic nanoclusters of a desired size, shape and composition on a well-defined substrate. In addition to high resolution electron microscopy (HRTEM), a new specialized STM/AFM technique is used to explore the surface morphology, size and shape of the bi(multi)metallic clusters, and the spatial atomic arrangement within the cluster. Monte-Carlo simulations of the equilibrium structure bimetallic nanoclusters are conducted using the embedded atom method (EAM). The relation between electrocatalytic function and microstructural characteristics is being established.

Major Program Achievements (over duration of support):
Shown that non-equilibrium bimetallic surface structures produced either by ion-implantation or by electrodeposition cannot be sustained during use as a polymer electrolyte membrane (PEM) fuel cell catalyst. HRTEM has shown that 2-5 nm bimetallic particles of Pt_3Sn do not have the ordered $L1_2$ ordered structure seen in larger (> 10 nm) particles. However, vibrational spectra of CO adsorbed onto 2-5 nm bimetallic particles of Pt_3Sn are identical to spectra from ordered Pt_3Sn bulk alloy surfaces. Monte-Carlo simulation of Pt-Re nanoparticles shows that surface segregation of Pt can produce a perfect "core-shell" equilibrium structure with no buried Pt atoms.

Program impact:
Demonstrated that a wide composition range for carbon supported bimetallic electrocatalysts must be employed to determine the optimum structure-composition. Commercial catalyst suppliers JM and TKK found enhanced activity for methanol electrooxidation after trying a wider range of compositions of Pt-Ru. Further optimization of carbon supported bimetallic electrocatalysts appears possible with improved understanding of the properties of bimetallic nanoparticles.

Interactions:
Michel Van Hove (Monte-Carlo simulation)
Mike Baskes (Sandia) potentials for the embedded atom method
H. Boennemann (M.P.I. Muelheim) nanoparticle synthesis
Prof. Klaus Wandelt (University of Bonn) STM/AFM
David Thompsett (JM, Johnson-Matthey) technology transfer
Tomoyuki Tada (TKK, Tanaka Kikinzoku Kogyo) technology transfer

Recognitions, Honors and Awards (at least partly attributable to support under this FWP):
Humbolt Foundation Fellowship (2002-04) to Matthias Arenz
2003 Olaf A. Hougen Lecture by Philip Ross, University of Wisconsin-Madison, September 2003
Invited Talk by Nenad Markovic, Gordon Research Conference on Fuel Cells, Newport RI, July 2003

Personnel Commitments for FY2003 to Nearest +/- 10%:
Philip Ross (P.I.) 20 %
Nenad Markovic (Scientist) 33 %
Michel Van Hove (Scientist) 10 %
Matthias Arenz (Postdoc) 100 % time to this project with partial support from Humbolt Foundation
Guo-Feng Wang (Postdoc) 100 %
Simun Mun (Scientist) 25 %

Authorized Budget (BA):
FY03 BA $237,000 FY04 BA $237,000 FY05 $212,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Mechanical and chemical properties of surfaces and interfaces
FWP Number: KC31

Program Scope:
Fundamental studies of surface structure, friction, lubrication, wear. Energy transfer in nanometer contacts. Atomic scale manipulation. Development of advanced atomic scale imaging and spectroscopy techniques: Scanning Tunneling and Atomic Force Microscopies (STM and AFM), High Pressure Photoelectron Spectroscopy (HPPES).

Major Program Achievements (over duration of support):
-Nanotriboloby: Discovered molecular scale friction mechanisms in lubricant monolayers. Determined molecular packing of alkyl-silanes, -amines and -alcohols (application to MEMS).
-Discovered unusual friction properties of Al-Ni-Co quasicrystals. Friction along periodic direction is 7 to 8 times higher than along non-periodic direction.
-Molecular manipulation: Determination of mechanisms of excitation of vibrations, rotations, dissociation and translations of single atoms and molecules during tip-substrate interactions.
-Discovered nature of H2 dissociation sites on Pd(111): contrary to traditional assumptions at least 3 neighboring vacancies needed (due to poisoning of Pd atoms by neighboring H atoms).
-Measuremed diffusion parameters of single CO molecules and CO-CO interaction energies.
-Structure of water on metals: diffusion, clustering and growth of water on metals. Theoretical determination (DFT) of structure and bonding of water in clusters on Pd(111).
-Demonstred existence of liquid-like layers on ice below 0C (premelting) and the influence of contamination by High Pressure Photoelectron Spectroscopy.
-Determined structure of catalyst surfaces under ambient pressure gas environments *in situ* during reaction by STM and by HPPES (applications to catalysis and environmental science). Examples: methanol oxidation reaction on Cu is determined by subsurface oxygen, only detectable in equilibrium with gas.

Program impact:
Provide insights into mechanisms of energy dissipation in friction, lubricant monolayers and their drainage under pressure (MEMS, Hard Disk lubes). Discovered unusual friction properties of quasicrystals (coatings applications). Enabled imaging of liquids with nanometer resolution (previously not possible). Enabled studies of catalysis and environmental science *in situ* using atomic resolution imaging and photoelectron spectroscopy.

Interactions:
Internal: Molecular Environmental Science project at ALS beam line 11. Surface Science and Catalysis (Gabor Somorjai). Molecular Foundry (Alivisatos, Frechet, Bokor, Louie, Bertozzi). External: AMES Laboratory: (tribology of quasicrystals). Sandia Natl. Lab. (Peter Feibelman, theory). Univ. Autonoma Madrid, Spain (STM theory). Ecole Normale Superieure Lyon, France (STM theory). Spanish National Research Council (tribology of monolayers). Univ. Barcelona, Spain: (organic monolayers, *ab-initio* calculations). Fritz-Haber-Institut Berlin, Germany: HPPES**.** University of Paris-VI: *ab-initio* calculations of chemisorption.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Fellow, American Vacuum Society. Keynote Speaker TNT Conference, Salamanca Spain. Keynote speaker at American Vacuum Society meeting, Urbana-Champaign, 2003. Plenary speaker in: Euronanoforum, Trieste, Italy, 2003; Nanotribology Workshop of the European Science Found., Portugal, Aug. 04; CECAM workshop on surfaces under high pressure, Lyon, France, Nov., 04; Nanospain Conf. March 05; TNT Oviedo, Aug. 05; Nanoscale Science & Techn. Workshop, Seattle, Sept. 05; 90th National Meeting of the Argentine Physics Association, Sept. 05.

Personnel Commitments for FY2003 to Nearest +/- 10%:
Staff: M. Salmeron (50%), D.F. Ogletree (20%). Postdocs: Jeong Park, (100%). Students: Evgeni Fomin, Mousslim Tatarkhanov, Tomoko Shimizu, Yabing Qi (100%), Admin: C. Ross (5%)

Authorized Budget (BA):
FY03 BA $405,000 FY04 BA $435,000 FY05 BA $421,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Femtosecond Dynamics in Condensed Matter
FWP Number: KC22

Program Scope:
This research program is focused on understanding fundamental dynamics in condensed matter on the ultrafast time scale. Electronic excitation, vibrational excitation, scattering, relaxation, and dephasing phenomena in novel solid-state systems and molecules are investigated on the 10 fs time scale using femtosecond pump-probe, photon echo, and transient anisotropy measurements with visible pulses.

Major Program Achievements (over duration of support):
This research program has demonstrated that carrier scattering and dephasing dynamics in semiconductors is strongly dependent on system dimensionality (degree of quantum confinement). In semiconductor nanocrystals, the polarization dephasing times (homogeneous linewidths) are mediated primarily by deformation coupling to acoustic modes, strongly enhanced by the quantum confinement. Our research has shown that electronic and vibrational dynamics of solvated molecules is strongly influenced by both steric and dielectric interaction with the solvent environment. The nature of the coupling to the solvent bath modes is manifest in the non-Markovian behavior in the dephasing of the optical polarization. In charge-transfer systems, steric interaction with the first solvent shell mediates the speed of the reaction. Our research has further demonstrated that fundamental chemical reactions (e.g. charge transfer reactions in organo-metallic molecules and isomerization reactions in rhodopsin chromophores) are nearly barrierless transitions that proceed along non-adiabatic potentials. Excited state dynamics in the Franck-Condon region play a critical role in determining the. photophysical properties of these systems. These results suggest a new paradigm for such ultrafast reactions in which the reaction proceeds from a vibrationally coherent (non-thermalized) excited state. Time-resolved x-ray diffraction studies in laser-heated semiconductors have revealed the first direct evidence of non-thermal melting. Ultrafast visible measurements of the optically induced insulator-metal transition in the correlated electron system, VO_2, reveals the transition is mediated by atomic structural changes, indicating that the band-like nature of the insulator state dominates over the Mott-Hubbard character. Studies of the insulator-metal transition in VO_2 nanocrystals reveal the dominant role of surface plasmon modes and points to potential technological applications. Recent measurements in the correlated-electron system $Pr_{0.7}Ca_{0.3}MnO_3$, reveal evidence of a phase-transition initiated via vibrational pumping of the Mn-O modes in the mid-infrared (~50 meV).

Program Impact: This program has elucidated a number of fundamental electronic and atomic dynamics in condensed matter systems. Result from semiconductors, solvated molecules, and correlated electron systems have challenged previously held assumptions and fostered new paradigms to describe the dynamic behavior. Ultimately these ultrafast dynamics substantially influence the material properties and functionality.

Interactions:
Internal—NERSC, Advanced Light Source, Accelerator and Fusion Research (Center for Beam Physics)
External—U.C. Berkeley Chemistry Department (A.P. Alivisatos, R. Mathies), U.C. Berkeley Physics Department (A. Zettle), Michigan State University (J. McCusker), U.C. Irvine Chemistry Department (S. Mukamel)

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
C.V. Shank - John Scott Award (Franklin Society, 1991)
R.W. Schoenlein – Adolph Lomb Medal (Optical Society of America, 1992)
C.V. Shank - George E. Pake Prize (American Physical Society, 1996)
C.V. Shank - Arthur L. Schawlow Prize in Laser Science (American Physical Society, 1997)
C.V. Shank - Charles H. Townes Medal (Optical Society of America, 2001)

Personnel Commitments for FY2004 to Nearest +/- 10%:
R.W. Schoenlein (50%), A. Cavalleri (35%), M. Rini Postdoc (100%)

Authorized Budget (BA):
FY03 BA $258,000 FY04 BA $258,000 FY05 BA $258,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Femtosecond X-ray Beamline for Studies of Structural Dynamics
FWP Number: KC22

Program Scope:
The application of x-ray techniques to study ultrafast structural dynamics such as phase transitions, chemical reactions, and surface processes on the fundamental time scale of a vibrational period (~100 fs) is an important new field of research in physics, chemistry, and materials science. The objectives of this research program are: (1) to develop a state-of-the-art research facility for time-resolved x-ray science based on a synchrotron beamline generating 100 fs x-ray pulses, (2) develop new time-resolved x-ray measurement techniques and instrumentation, and (3) address fundamental scientific questions related to atomic and electronic structural dynamics in condensed matter using time-resolved diffraction and spectroscopy techniques with femtosecond x-ray pulses.

Major Program Achievements (over duration of support):
This research program has provided the first demonstration of femtosecond pulses generated from a synchrotron. The femtosecond x-ray flux and background levels have been characterized and compared with model calculations. This research program has supported the development of a bend-magnet beamline and instrumentation at the ALS for time-resolved measurements including a sub-picosecond x-ray streak camera with photoconductive trigger. Time resolved x-ray spectroscopy measurements in the correlated electron system, VO_2, have revealed the sub-picosecond dynamic shift of the vanadium L_{III}-edge associated with the optically induced insulator-metal transition. These results represent the first application of femtosecond x-ray spectroscopy. Time-resolved diffraction measurements in the ferroelectric crystal LiTaO3 reveal the coherent vibrational dynamics of the phonon-polariton mode (~350 fs period) and enable the direct measurement of associated atomic displacements for the first time. Time-resolved EXAFS and XANES measurements in transition-metal spin-crossover molecular complexes (Fe^{II}) reveal a 0.2 Å dilation of the Fe-N bond distance developing within 70 ps. This is the first dynamic measurement of the structural changes associated with the photo-induced formation of the high-spin state.

Program Impact:
This program is a leading contributor to the development of the new research area of femtosecond x-ray science.

Interactions:
Internal - LBNL Chemical Sciences Division (A. Belkacem), Advanced Light Source, LBNL Accelerator and Fusion Research Division (Center for Beam Physics)
External - U.C. Berkeley Physics Department (R. Falcone), Michigan State University (J. McCusker), Univ. of Lausanne (M. Chergui, C. Bressler). University of Tokyo (S. Koshihara), U.C Irvine (S. Mukamel)

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
R.W. Schoenlein – Klaus Halbach Award (Advanced Light Source, 2000)
R.W. Schoenlein – Program Committee, Ultrafast Phenomena Conference (1998-present)
A. Cavalleri – Shirley Prize for Outstanding Scientific Achievement (Advanced Light Source, 2004)
A. Cavalleri – European Young Investigator Award (European Science Foundation, 2004)

Personnel Commitments for FY2005 to Nearest +/- 10%:
R.W. Schoenlein (50%), A. Cavalleri (40%)

Authorized Budget (BA):
FY03 BA $257,000 FY04 BA $270,000 FY05 BA $145,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Experimental Solid State Physics and Quantum Electronics
FWP Number: KC22

Program Scope: Development of novel nonlinear optical spectroscopic techniques to study materials and explore new areas of material science. Sum-frequency spectroscopy, in particular, is developed as a surface-specific tool and used to study polymer interfaces, liquid/liquid interfaces, water/oxide interfaces, surface reactions and dynamics, electrochemical interfaces, molecular conformation at interfaces, biomolecules adsorbed at interfaces, and molecular chirality.

Major Program Achievements (over duration of support):
Established the field of surface nonlinear optics by work on surface-enhanced nonlinear optical effects, nonlinear optics with surface waves, and surface second-harmonic and sum-frequency generation. Pioneered cross laser-molecular beam studies with Y.T. Lee. Developed optical second-harmonic and sum-frequency spectroscopy into a powerful and versatile surface analytical tool. Found unique applications of the spectroscopic technique on many important surfaces and interfaces such as those of water, polymers, ice, and many other liquids and solids, and obtained fundamentally interesting, but hitherto unavailable, results on such interfaces. Demonstrated in collaboration with G.A. Somorjai, the use of sum-frequency spectroscopy as a unique tool to study surface reactions under ambient conditions and polymer surfaces and interfaces. Also developed a new powerful optical technique to study surface chemical diffusions of atoms and molecules that allows sensitive probing of anisotropy, concentration dependence, impurity effect, etc. in surface diffusion. Established sum-frequency generation as a novel sensitive spectroscopic tool to probe molecular chirality. Study of chiral biological molecules *in situ* and development of chiral sum-frequency microscopy for imaging of real biological systems are in progress.
Program Impact:
Developed novel laser techniques that have attracted much interest in the material science and chemical physics communities. Created a new research area of surface nonlinear optics in quantum electronics and surface science. The surface nonlinear optical spectroscopy technique developed in our laboratory has become a widely known surface analytical tool adopted by many surface science laboratories. Our experimental setup served as a prototype for several commercial systems.

Interactions:
Internal: Mat. Sci. Div. (M.Salmeron, G.A.Somorjai, P.Ross): Earth Sci. Div. (G.Waychunas)
External: Berkeley campus (R. Saykallay, H. Yang, X. Zhang); Inst. of Atomic and Molecular Sci., Acad. Sinica, Taiwan (M.Hayashi, S.H.Lin); Wietzmann Inst. (L. Leiserowicz); Naval Res. Lab. (D. Shenoy); Japan Sci. & Tech. Corp, Japan (M. Oh-e); Tokyo Inst.Tech., Japan (S. Koshihara)
Recognitions, Honors, and Awards
C.H..Townes Award, Opt. Soc.Am.,(1986); A.L.Schawlow Prize, Am. Phys. Soc.,(1992); Distinguished Traveling Lecturer, Laser Sci. Group of APS(1994-96); Max Planck Int. Research Award(1996); Chancellor's Prof. at Berkeley(1997-2000); Mat. Sci. Award in Sol. St. Phys., Significant Implication for DOE Related Technology(1997); D.Sc, Honoris Causa, Hong Kong Univ. of Sci. and Tech., HK,(1997) and Nat. Chao Tung Univ., Taiwan(1998); F. Isakson Prize, APS(1998); Member, Nat. Acad. of Sci(1995)., Amer. Acad. of Arts and Sci.(1990), Acad. Sinica(1990)., Foreign member, Chinese Acad. of Sci.(1996); Honorary Chair Professor, Nat. Tsing Hua Univ., Taiwan (2001-2007). Approx. 30 invited talks in the last three years.

Personnel Commitments for FY2005 to Nearest ±10%
Y.R. **Shen**, (Group leader) 50%; J.McGuire (Student) 50%; Ji Na (Student), 50%,; L. Zhang (Student) 50%, partly paid by U.C.; T. Troung (Student) 50%, paid by U.C.; W.T.Liu, 50% (Student), paid by UC; K.Ikeda (Visiting Scientist), 100%, supported by Japanese fellowship.. F. Wang, 100%, supported by U.C.

Authorized Budget (BA):
FY03 $326,000 FY04 $226,000 FY05 $326,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP:
Spin Functionality through Complex Oxide Heteroepitaxy

FWP Number: KC12

Program Scope: Development of highly spin polarized thin film materials that will shed light on key unresolved questions in magnetism concerning the nature of magnetism at boundaries of spin-polarized materials and that will facilitate more energy efficient spin-based electronic applications. We are developing novel functional oxide thin films and heterostructures with spin polarized functionality in order to: (i) design and synthesize complex oxide thin film materials with spin polarized functionality; (ii) obtain a fundamental understanding of the nature of magnetism at boundaries; (iii) develop close collaborations with colleagues at Lawrence Berkeley National Lab (LBNL), Argonne National Laboratory (ANL) and other DOE labs; (iv) act as a resource for thin film materials development; (v) train the next generation of scientists in thin film materials synthesis at the undergraduate, graduate and postdoctoral levels.

Major Program Achievements (over duration of support- July to September 2005):
Ordered perovksites: Developed layered manganite thin films with the layers perpendicular to the substrate. These types of films have elucidated the anisotropy of the magnetism and transport in these layered materials that has not been easily measured in bulk single crystal samples.

Oxide junction heterostructures: Developed oxide junction heterostructures based on oxide spinels and perovskites. These junctions show that ferromagnetic Fe_3O_4 is negatively spin polarized and exhibit junction magnetoresistance values of up to -25%. Bias and magnetic field dependence of the junction transport reveal that the transport is a combination of direct tunneling and hopping through localized states.

Novel oxide interface materials: Developed thin film processing methods to synthesize oxide thin films with rms surface roughness on the order of one unit cell.

Program Impact:
The development of complex oxide thin film materials with spin polarized functionality has provided model systems which shed light on the nature of magnetism at boundaries of spin-polarized materials. Understanding spin polarization at these surfaces and interfaces is a key element in the development of a more energy efficient spin-based electronics.

Interactions:
Argonne National Laboratory, Materials Science Division: J.F. Mitchell, H. Zheng
Stanford University, Laboratory for Advanced Materials, A.F. Marshall
Norwegian University of Science and Technology, Department of Electronics and Telecommunication, J.K. Grepstad

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
None from July 2005 for a total of 3 months for FY2005
2005 Maria Goeppert Mayer Award, American Physical Society to Y. Suzuki.

Personnel Commitments for FY2005 to Nearest +/-10%:
Note that funding started July 2005 for a total of 3 months for FY2005
Y. Suzuki (PI) 20% time for this project but paid for 0% time as funding spending began in August 2005
Y. Takamura (post-doc) 100%
B.B. Nelson-Cheeseman 100% time this project but paid for 0% time by DOE as she is on fellowship

Authorized Budget (BA):
FY03 BA $0 FY04 BA $0 FY05 BA $250,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020203

FWP and/or subtask Title under FWP:
Predicting the Electronic Properties of 3D, Million-Atom Semiconductor Nanostructure Architectures

FWP Number: KC31

Program Scope: To develop new computational approaches for thousand atom nanostructure calculations. Especially to develop the charge patching method, so the electronic structures and optical properties of thousand atom nanocrystals can be calculated with ab initio accuracy, replacing the empirical pseudopotential method, also to calculate the electronic structures of multicomponent nanostructure architectures.

Major Program Achievements (over duration of 2004-2005):
Finished the motif polarization coding and testing: we have implemented and tested the way to use charge motifs to represent the polarization response of a nanosystem to an external electric field. The charge response (polarization) to an electric field calculated using the polarized motif is very close (including the local field effects) to the one calculated directly using selfconsistent ab initio calculations. This new scheme will significantly enlarge the applicability of the charge patching method. Now, systems with long range electric field (e.g, quantum dots with dipole moments, charged impurities, charged quantum dots) can be calculated.

Ab initio accuracy quantum dot and quantum wire calculations: We have used the charge patching method to calculate the optical band gaps of quantum dots and wires of thirteen different semiconductor materials. For systems experimental data exist, our results agree well with experiments. For systems experimental data do not exist, our results serve as benchmarks for future calculations and experiments.

6000 atom nano-dumbbell calculations: Using the charge patching method, we have calculated a nano-dumbbell consisted with two CdTe balls connected by a central CdSe wire (multicomponent nanostructure). Many-body effects among the carriers are calculated, and charge localizations are studied. It is demonstrated that by controlling the width of the CdSe wire, one can control the localization of the electron state.

Quantum dot/quantum well system: We have calculated the CdS/CdSe/CdS quantum dot/quantum well nanosystem. Experimentally quantum dot/well systems have been synthesized. Such systems can provide large geometry variational space to control its electronic properties. Theoretical study and understanding can help the rational design of such systems to provide the desired properties.

Surface polarization effects on a nanostructure: We have derived the electron Schrodinger's equation in a nanostructure including the surface polarization potential. This equation was derived 20 years ago based on classical electrostatic arguments. We have now derived it from the many-body GW equation. We have also used this equation to study the charging effects of an nano-tetrapod, and pointed out the importance of the surface polarization term.

A general charge patching scheme: We have been working on a generalized charge patching scheme, which can include one atom motifs and multiple atom (cluster) motifs. The idea is to put together the charge densities from various prototype calculations, some from bulk systems, some from molecules, or impurity containing regions. This will provide more flexibility for the charge patching method in nanoscience calculation.

A bulk-band preconditioner: We have developed a preconditioner for the conjugate gradient scheme in solving the single particle Schrodinger's equation. This preconditioner is derived from the bulk states and can speed up the convergence by a factor of 5.

Program Impact:
The development of the charge patching method enables us to calculate thousand atom nanosystems with ab initio accuracy. The calculation is fast and scales linearly to the size of the system.

Interactions:
National Renewable Energy Lab: (A. Zunger). Univ. of Tennessee: (Jack. J. Dongarra).

Personnel Commitments for FY2003 to Nearest +/-10%:
Lin-Wang Wang 15%
Joshua Schrier (post-doc) 100%
Authorized Budget (BA):
FY03 BA $90,000 FY04 BA $175,000 FY05 BA $165,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Multi-component assembly of high surface-area ordered oxide-metal nanocomposites with enhanced catalytic properties.
FWP Number: KC31

Program Scope: Developing novel synthetic strategies for shape-controlled growth of Au, Pt and bimetallic nanocrystals, ideally with one type of surface exposed only; 2-dimensional assembly of these nanocrystals using Langmuir-Blodgett technique; 2- and 3-dimensional Assembly of these shaped nanocrystals within ordered porous oxide (SiO_2, Al_2O_3, TiO_2) matrix; Chemical reaction testing on the ordered metal-oxide nanocomposites to examine the effect of surface type of the nanocrystals, interface and surface area on the catalytic activity and selectivity.

Major Program Achievements (over duration of support):
(1). We have successfully synthesized monodisperse Pt nanocrystals with three different shapes – cubes, cuboctahedra, and octahedra selectively with similar sizes of 9 ~ 10 nm by a modified polyol process. We found that addition of silver ion enhances the crystal growth rate along <100>, and essentially determines the shape and surface structure of the Pt nanocrystals. 2-dimensional ordered array of the Pt nanocrystals were assembled by Langmuir-Blodgett (LB) method. The particles were evenly distributed on the entire substrate, and their surface coverage and density can be precisely controlled by tuning the surface pressure. The resulting Pt LB layers are potential candidates for 2-dimensional model catalysts due to their high surface area and structural uniformity of the metal nanocrystals.
(2). Thermal stability of facetted Pt nanocrystals on amorphous silica support films was investigated using in-situ transmission electron microscopy in a temperature range between 25 and 800 °C. The particles started to change their shapes at ~350 °C. Above 500 °C, the particles spread on the support film with increasing temperature, rather than becoming more spherical. Such temperature-induced wetting of Pt nanoparticles on silica surface can be attributed to the interfacial mixing of Pt and SiO_2 and the resulting negative interface energy.
(3). A novel high surface area heterogeneous catalyst based on solution phase colloidal nanoparticle chemistry has been developed. Monodisperse platinum nanoparticles of 1.7-7.1 nm have been synthesized by modified solution based alcohol reduction methods and incorporated into mesoporous SBA-15 silica during hydrothermal synthesis. Characterization of the Pt/SBA-15 catalysts suggests that Pt particles have been incorporated into the internal structure of the silica. After removal of the templating polymer from the nanoparticle surface by thermal calcination and reduction, Infrared studies of CO adsorption revealed that CO predominantly adsorbs to atop sites and red shifts as the particle size decreases suggesting surface roughness increases with decreasing particle size. Ethylene hydrogenation and ethane hydrogenolysis were chosen to test for catalytic activity and size-dependent catalytic behavior, respectively. Ethane hydrogenolysis displayed significant structure sensitivity over the size range of 1–7 nm, while the apparent activation energy increased linearly up to a Pt particle size of ~ 4 nm and then became constant. The observed rate dependence with particle size is attributed to a higher reactivity of coordinatively unsaturated surface atoms in small particles compared to highly coordinated atoms in low index surfaces prevalent in large particles.

Program Impact:
Enabling the deterministic assembly of high surface-area oxide-metal nanocomposites with enhanced catalytic activity and selectivity (i.e. catalyst-by-design).

Interactions:
G. Somorjai (Chemistry): Catalytic reaction studies on the high surface-area ordered metal-oxide nanocomposites.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2005, ACS Pure Chemistry Award.

Personnel Commitments for FY2003 to Nearest +/-10%:
P.D. **Yang** (PI) 20%**;** H. Song (postdoc) 100%; Susan Habas (graduate Student) 100%

Authorized Budget (BA):
FY03 BA $195,000 FY04 BA $195,000 FY05 BA $195,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Nanowire-Based Functional Devices and Assemblies
FWP Number: KC12

Program Scope: Vapor-liquid-solid (VLS) process will be used to grow monocrystalline nanowires Si, Ge, SiGe, GaN, ZnO and various II-VI semiconductors. Significant research efforts will be placed on the fundamental understanding of the nanowire nucleation/growth. The fundamental information will then be used to guide the nanowire growth process which would include monodispersity control over size and aspect ratio; growth orientation control, precise site control and accurate density control. Lastly, both parallel process (Langmuir-Blodgett technique) and serial process (nanomanipulation) will be explored for the hierarchical assembly of these nanowire building blocks for their potential nanoelectronic and nanophotonic applications.

Major Program Achievements (over duration of support):
(1). Control over the nanowire growth direction is extremely desirable, in that anisotropic parameters such as thermal and electrical conductivity, index of refraction, piezoelectric polarization, and bandgap may be used to tune the physical properties of nanowires made from a given material. We have demonstrated the use of metal−organic chemical vapour deposition (MOCVD) and appropriate substrate selection to control the crystallographic growth directions of high-density arrays of gallium nitride nanowires with distinct geometric and physical properties. Epitaxial growth of wurtzite gallium nitride on (100) γ-$LiAlO_2$ and (111) MgO single-crystal substrates resulted in the selective growth of nanowires in the orthogonal $[1\bar{1}0]$ and [001] directions, exhibiting triangular and hexagonal cross-sections and drastically different optical emission. The MOCVD process is entirely compatible with the current GaN thin-film technology, which would lead to easy scale-up and device integration.
(2). Although the electrical integration of chemically synthesized nanowires has been achieved with lithography, optical integration, which promises high speeds and greater device versatility, remains unexplored. We have explored the properties and functions of individual crystalline oxide nanoribbons that act as subwavelength optical waveguides and assess their applicability as nanoscale photonic elements. The length, flexibility, and strength of these structures enable their manipulation on surfaces, including the optical linking of nanoribbon waveguides and other nanowire elements to form networks and device components. We have demonstrated the assembly of ribbon waveguides with nanowire light sources and detectors as a first step toward building nanowire photonic circuitry.
(3). The manipulation of optical energy in structures smaller than the wavelength of light is key to the development of integrated photonic devices for computing, communications and sensing. We have assembled small groups of freestanding, chemically synthesized nanoribbons and nanowires into model structures that illustrate how light is exchanged between subwavelength cavities made of three different semiconductors. Using simple coupling schemes, lasing nanowires can launch coherent pulses of light through ribbon waveguides that are up to several millimeters in length. In addition, we found that nanoribbons function excellently as waveguides in liquid media and provide a unique way to probe molecules in solution or in proximity to the waveguide surface. Our results lay the spadework for photonic devices based on assemblies of active and passive nanowire elements and presage the use of nanowire waveguides in microfluidics and biology.

Program Impact: Develop the science and technology of a broad spectrum of 1-dimensioanl inorganic semiconducting nanostructures or nanowires for energy-related applications including nanophotonics and energy conversion.

Interactions: Arun Majumdar; Ali Shakoli(UCSC, Mechanical Engineering), Kaiming Ho (Iowa State. Physics)
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2005, ACS Pure Chemistry Award.
Personnel Commitments for FY2003 to Nearest +/-10%:
P.D. **Yang** (PI) 20%**;** B. Yuhas (Graduate student) 100%; Don Sirbuly (Postdoc) 100%; Iowa State: Xinhua Hu (postdoc 0.5), Zhuo Ye (graduate student); UCSC: Yan Zhang, James Christofferson (Graduate Students)

Authorized Budget (BA):
FY03 BA $ 0 FY04 BA $ 0 FY05 BA $411,000

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Novel sp^2-bonded Materials
FWP Number: KC31

Program Scope:
Ab-initio quantum mechanical calculations to predict new materials structures and relate them to electronic structure and mechanical and thermal properties. Experimental synthesis of novel sp2-bonded materials including functionalized nanostructures, and characterization using SEM, TEM, STM, AFM, XRD, mechanical properties, and transport properties. Nanoscale device fabrication and testing. Strong connection between theory and experiment.

Major Program Achievements (over duration of support):
Prediction of new nanostructures including BxCyNz, CN, and GaSe nanotubes and nanoparticles. Theoretical analysis of nanotube hybrid structures (e.g. peapods) and devices. Tuning of the bandgap of BN nanotubes and doping of carbon nanotubes studied theoretically and experimentally. Successful experimental synthesis of BN double-walled nanotubes and nanococoons, nanotube rectifiers, matrix field emission sources, n- and p-type nanotube transistors, and crossed tube devices. Thermopower and thermal conductivity of nanotubes and nonlinear conductance of nanotubes determined theoretically. Nanobearings fabricated from nanotubes and frictional properties determined. Young's modulus of carbon and BN nanotubes determined. Electron holography of field-emitting nanotube performed. Oxygen sensitivity of nanotubes discovered. New fullerene-like materials synthesized. High resolution, low temperature UHV STM studies of BN nanotubes and carbon nanotube junctions and fullerenes performed. Zone-refinement of carbon nanotubes. High resolution STM studies of nanotubes and fullerenes.

Program impact:
First experimental demonstration of nanotube electronic device and nanotube nanobearing. First demonstration of nanotube chemical sensor. Discovery of BN nanotubes, silocrystals and nanoparticles. First STM studies of BN nanotubes. Experimental verification of Giant Stark Effect in BN nanotubes. Controlled charge state of individual C60 molecule through reversible single-atom doping. Mapped electronic structure of fullerenes and phase diagram of doped C60 molecular layers.

Interactions:
Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory
External: University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, SUNY Stony Brook, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Alex Zettl – LBNL Outstanding Performance Award 2004, R&D 100 Award 2004, 33 invited talks since 2003.
C. Bertozzi - Elected to the National Academy of Sciences in May 2005, 91 invited talks since 2003.
M. L. Cohen –U.S. National Medal of Science; ISI's top 100 most-cited physicists; President of the American Physical Society; member of American Philosophical Society; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Harvard University Loeb Lecturer; University of Montreal Doctorat Honoris Causa; 43 invited talks since 2003.
S. G. Louie –APS Davisson-Germer Prize; ISI's top 100 most-cited physicists; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Outstanding Overseas Chinese Award; member of National Academy of Sciences; 48 invited talks since 2003.
M. Crommie – 10 invited talks since 2003.

Personnel Commitments for FY2005 to Nearest +/- 10%:
PI's (Zettl 25%, Bertozzi 10%, Cohen 25%, Louie 20%); Visiting Scientist: (Capaz, - fellowship 50%); Post Docs (Son 75%, Kirakosian 100%, Wiachwiak 100%, Kis 100%, Ikuno 50%, Regan 20%,); GSR's (Khoo 50%, Luo 50%, Fennimore 50%, Mickelson 50%, Begtrup 25%, Yuzvinsky 25%, Chang 25%, Jensen 25%, Girit 25%, Kessler 25%, Huang 25%, Comstock 50%, Chen 50%)

Authorized Budget (BA):
FY03: $602,000 (sp2) + $611,000 (FuncNano) + $569,000 (Xtal) = $**1,782,000**
FY04: $456,000 (sp2) + $499,000 (FuncNano) + $570,000 (Xtal) = $**1,525,000**
FY05: $456,000 (sp2) + $434,000 (FuncNano) + $364,000 (Xtal) = $**1,254,000**